Exact solutions in the FPU oscillator chain

P. Poggi[1] S. Ruffo[1,2*]

[1] *Dipartimento di Energetica, Università di Firenze, via S. Marta 3, I-50139 Firenze (Italy).*

[2] *INFN and INFM, Firenze (Italy).*

16 October 1995

Abstract

After a brief comprehensive review of old and new results on the well known Fermi-Pasta-Ulam (FPU) conservative system of N nonlinearly coupled oscillators, we present a compact linear mode representation of the Hamiltonian of the FPU system with quartic nonlinearity and periodic boundary conditions, with explicitly computed mode coupling coefficients. The core of the paper is the proof of the existence of one-mode and two-mode exact solutions, physically representing nonlinear standing and travelling waves of small wavelength whose explicit lattice representations are obtained, and which are valid also as $N \to \infty$. Moreover, and more generally, we show the presence of multi-mode invariant submanifolds. Destabilization of these solutions by a parametric perturbation mechanism leads to the establishment of chaotic in time mode interaction channels, corresponding to the formation in phase space of bounded stochastic layers on submanifolds. The full mode-space stability problem of the $N/2$ zone-boundary mode is solved, showing that this mode becomes unstable through a mechanism of the modulational Benjamin-Feir type. In the thermodynamic limit the mode is always unstable but with instability growth rate linearly vanishing with energy density. The physical significance of these solutions and of their stability properties, with respect to the previously much more studied equipartition problem for long wavelength initial excitations, is briefly discussed.

PACS numbers: 05.45.+b, 63.20.Ry, 63.10.+a

Keywords: Anharmonic lattices; Energy equipartition; Periodic solutions; Hamiltonian bifurcations; Stochastic layers.

*e-mail: ruffo@ingfi1.ing.unifi.it

1 Introduction

The numerical experiment by Fermi, Pasta, Ulam (FPU) and Tsingou[1] [1], perhaps the first of all times, was the first attempt to check the predictions of classical statistical mechanics concerning the dynamics of a Hamiltonian system of coupled oscillators with a large number N of degrees of freedom. The result of this experiment was a big surprise: the expected relaxation to equipartition of energy among the linear normal modes was not revealed, during the time of observation and with low energy initial excitations. This also implies that ergodicity is not an obvious consequence of the non-existence of analytic first integrals of the motion besides the total energy (and possibly total momentum). After an initial growth of the energy in the neighbouring modes (as expected) they observed that the energy sharing was restricted only to the first modes, with a quite regular dynamics, rather than detecting a gradual and continuous energy flow from the first excited mode to the higher ones and a stochastic dynamics. Even more surprisingly, at later times, almost all the energy was flowing back into the initially excited mode, so that the system seemed to possess quasiperiodicity properties. Chirikov et al. [2] showed later, also with numerical experiments [3], that, at sufficiently high energies, the FPU model did relax to the equipartition state, on times which become smaller and smaller as the energy is increased. It then became clear that such a system was displaying qualitatively different behaviours as the energy, fixed by the initial condition, was varied. Chirikov and Izrailev [2] gave also the first linear normal modes representation of the system and applied the nonlinear resonances theory to predict the existence of the transition between the two behaviours. They did also recognize the resemblance between these results and the Kolmogorov-Arnol'd-Moser [4] theorem, first formulated, although not completely demonstrated, by Kolmogorov just in the same year of the FPU numerical experiment. These results successively stimulated a lot of numerical studies aiming at determining the dependence of the different observed behaviours of the FPU system on the number N of degrees of freedom (see Ref. [5] and references cited therein, and also [6, 7, 8, 9]).

It is now well established that the transition between a quasi-integrable behaviour to a mixing one, in the FPU system as well as in similar models (Lennard-Jones in 1-D and 2-D, ϕ^4), is controlled by the energy. At small energies the motion is weakly chaotic with positive but small Lyapunov exponents, revealing the presence of thin stochastic layers in the phase space, which is mostly filled with KAM tori. At higher energies the maximum Lyapunov exponent and the Kolmogorov-Sinai entropy rise considerably, revealing the growth of stochastic regions. In this energy range the temporal signals of normal mode energies also become chaotic. Well above the transition region all the signatures of large-scale chaos are present, with $N-1$ ($N-2$ for systems with periodic

[1] M. Tsingou contributed to the numerical work and then did not participate in the writing of the report.

boundary conditions) positive Lyapunov exponents, fast diffusion of the orbit over the constant energy surface, rapidly decaying spatio-temporal correlation functions (also between the modal energies). It has been also shown [10] that, in this region, a density function of Lyapunov exponents can be introduced in the thermodynamic limit, which can also be analytically estimated with a random matrix approximation [11].

On the other hand, the quasiperiodic behaviour at low energy was interpreted in terms of a continuum limit of the model. It was in fact observed by Zabusky and Kruskal [12] that, increasing the number N of oscillators while holding constant the length of the chain, the FPU model with cubic nonlinearity can be reduced to the Korteweg-deVries (KdV) equation in the limit of low amplitude and long wavelength excitations, after selecting one of the two possible directions of propagation for travelling waves. For the KdV equation the same authors found numerically the existence of localized solutions which preserve their shape even after mutual collisions. To emphasize the extremely stable and localized character of such solutions Zabusky and Kruskal called them *solitons*. It was shown later [13, 14, 15] that the KdV equation is a completely integrable infinite-dimensional Hamiltonian system, whose initial value problem can be solved by the spectral tranform method [16, 17]. The quasiperiodic behaviour of the FPU system at low energies is consequently believed to be the result of the presence on the lattice of several solitons emerging from the long wavelength initial condition and travelling with different speeds so that, at particular times, they reproduce almost exactly the initial condition. Quasiperiodic behaviour is destroyed at larger energies, above the threshold of transition to equipartition [6]. A deeper understanding of this transition phenomenon requires a systematic study of its dependence on the number of degrees of freedom, on the initial condition and on the time of observation. Such a study has not been fully completed yet.

1.1 The FPU model

The FPU system is an approximate model for the behaviour of a classical solid at low temperatures. The reduction of complexity in comparison to the real physical situation is considerable. First of all only one spatial dimension is considered and then the interaction (typically of the Lennard-Jones kind) is expanded in the small displacements around the equilibrium positions of the atoms or molecules, i.e. the weakly anharmonic case is considered (in practice the case of rather low temperatures). As a consequence, several problems must be discussed concerning the physical relevance of the FPU model. We must first ask if the observed phenomena are peculiar of the model or can be instead revealed in a wider class of more physical models. This issue is now clarified and we can state with no doubt that different models in one and two dimensions share the same phenomenology (see Ref. [5] for a review). In particular, practically all the models which, as the FPU one, are constituted by weakly coupled anharmonic oscillators, show the prevalence of ordered motion

at sufficiently low energies, while at higher energies their phase space becomes chaotic. An important point is that the transition between the "ordered" region and the "chaotic" one happens in an energy range relevant for physics. For example, in a model of oscillators in two dimensions with Lennard-Jones interactions [18], the transition, with the physical parameters of Argon, is found to happen around a temperature of 5 $^\circ K$. Some recent molecular dynamics calculations [19] on a model for a Xenon crystal with diluted impurities made of Iodine molecules, show that the time required for the equipartition of energy between the initially excited I_2 molecule and the Xe matrix abruptly increases at approximately 30 $^\circ K$; such a physical situation could be investigated in a real experimental sample.

Having established the physical relevance of the phenomena studied in the FPU model, we proceed to its definition. The FPU model is a one-dimensional chain of oscillators with unit mass, with weakly nonlinear nearest-neighbour interaction (the lattice spacing is also taken of unitary length). Calling q_i and p_i the coordinates and, respectively, the momenta of the oscillators, the model is defined by the following Hamiltonian:

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=1}^{N} \left[\frac{1}{2}(q_{i+1} - q_i)^2 + \frac{\beta}{r}(q_{i+1} - q_i)^r \right] , \tag{1}$$

where $q_1 \equiv q_{N+1}$ and $r = 3$, for the so-called FPU-α model, while $r = 4$ for the FPU-β model. We consider in the present work only the FPU-β model, with periodic boundary conditions to allow travelling wave solutions (whereas in the original FPU paper fixed ends boundary conditions were chosen). At fixed energy, the coupling constant β determines the amount of nonlinearity in the model. Conversely, as it is more natural, for a fixed β the increasing departure from the harmonic behaviour is controlled increasing the energy. It can be easily shown that the dynamics depend only on the parameter $\beta E^{(r/2-1)}$, where E is the total energy, fixed by the initial condition.

Hamiltonian (1), written in linear normal coordinates (Q_k, P_k) (phonons) becomes

$$H = \frac{1}{2} \sum_k \left(P_k^2 + \omega_k^2 Q_k^2 \right) + \beta V(\boldsymbol{Q}) \ . \tag{2}$$

with frequencies $\omega_k = 2\sin(\pi k/N)$ in the case of periodic boundary conditions (the harmonic frequency spectrum is obvioulsy different from the case of fixed boundary conditions studied by FPU) and we have $\omega_k = \omega_{N-k}$, so that there are only $N/2$ different frequencies (if N is even, for simplicity). The harmonic energy of mode k is defined by $E_k = (P_k^2 + \omega_k^2 Q_k^2)/2$.

The FPU experiment aimed at showing the progressive decorrelation of the system during its temporal evolution, eventually leading to ergodic behaviour. To this end they chose an initial condition far from equilibrium, giving all energy to the lowest ($k = 1$) normal mode only, and then calculating the instantaneous

energies $E_k(t)$ of all modes. They expected to see a progressively uniform redistribution of energy between all modes, caused by the small anharmonic coupling between them. On the contrary they observed the well known FPU recurrent behaviour: energy was flowing back regularly to mode $k = 1$ after an initial share. Return to the initial condition is not exact, but the possibility that relaxation is present on longer times was ruled out by the numerical experiment of Tuck and Menzel [20], who first observed the "superperiod" phenomenon.

The behaviour of average energies $\bar{E}_k(T) = T^{-1} \int_0^T E_k(t)dt$ versus T, shows that the systems relaxes to an asympotic state, but the latter is different from that in which equipartition of energy holds. On the contrary, at higher energy [3], the equipartition state is reached in a relatively short time. A transition is present from an "ordered" state, in which the system seems not to be relaxing towards equipartition, showing recurrent behaviour in time, to a different one where, on the contrary, equipartition is quickly reached, which we call a "chaotic" state (though these terms are improper because also in the "ordered" state there are chaotic solution, but they fill a part of small measure in the phase space).

Various indicators have been employed to characterize this transition, either based on the distribution of energy among the normal modes [7], or on the local divergence rate of nearby trajectories in phase space (Lyapunov exponents) [18]. In particular, the first clear numerical evidence of the transition to equipartition (or "chaotic") state was obtained in Ref. [6] by the use of an appropriate Shannon entropy S defined in the space of modes ("spectral entropy"). At a given value of the control parameter

$$\epsilon = \frac{\beta E}{N} \ , \tag{3}$$

where E is the total energy, the "spectral entropy" was shown to increase, reaching then its maximal value.

Despite these results the problem is still far from beeing understood, especially concerning the dependence of the phenomenology on the number of degrees of freedom and on the time scales of observation.

1.2 Recent results

We will focus on the results which are valid at large N (thermodynamic limit). The first result we want to mention concerns the Lyapunov spectrum well above the region of transition to equipartition ($\epsilon \gg 1$). There are strong numerical evidences [10] supporting the possibility to define a function $\phi(x)$ which represents the density of Lyapunov exponents in the thermodynamic limit, in the case when the only vanishing exponents are those related to space and time translational symmetries (momentum and energy conservation, respectively). After labelling the Lyapunov exponents in the decreasing order $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{2N}$,

the density function $\phi(x)$ is given by

$$\phi(x) = \lim_{N\to\infty} \lambda_{xN}(N) \ . \tag{4}$$

The existence of this limit was conjectured by Ruelle [21] for the Navier-Stokes equation, and verified by Manneville [22] for the Kuramoto-Sivashinsky equation. The existence of such a function makes it possible to define (using the Pesin relation) the Kolmogorov-Sinai entropy as an intensive quantity in the thermodynamic limit, thus proving the persistence of a state of large-scale chaos also when the number of degrees of freedom goes to infinity. So, when the intensive control parameter ϵ is big enough, the trajectory of the system visits in a short time all accessible regions of phase space and, as a consequence, equipartition of energy among the normal modes is quickly reached. The evidence for the existence of the Lyapunov exponents density function shows, in an indirect way, that equipartition of energy in the FPU model occurs also in the thermodynamic limit, when the energy density is high enough. Unfortunately there are no analytical results proving the existence of the function $\phi(x)$, apart from those obtained by Eckmann and Wayne using a random matrix approximation [11]. A recent discussion of this problem was also given by Sinai [23], who has indeed obtained a rigorous proof of the existence of an analogous quantity, obtained interchaning the order of the limits $N \to \infty$ and $t \to \infty$ (the latter appearing in the definition of the Lyapunov exponents). Though this is not, a priori, the same thing as ϕ, it can be argued [23] to be more relevant for statistical mechanics; moreover it has a closer correspondence to the numerical procedures used to determine ϕ.

Pettini and Landolfi [8] found a rapid decrease of the maximum Lyapunov exponent λ_1 as the control parameter ϵ is decreased below a value $\epsilon \approx 0.1$; such a behaviour does not change significantly when N is increased. Even if this does not necessarily prove the onset of large-scale chaos (because only a few directions, among many, might be responsible for the increase of the divergence rate), the persistence of the result when N is varied reveals the presence of an important phenomenon occurring in phase space. This result is consistent with the results obtained using the "spectral entropy", which also sharply increases around $\epsilon \approx 0.1$ (although a slower diffusion of the entropy with time is also present for smaller values of ϵ) [24, 25, 26].

More recently [27] it has been suggested that the largest Lyapunov exponent can be estimated from the temporal evolution of the vector $\boldsymbol{\xi}$ representing the deviation between geodesics on the Riemannian manifold constructed with the Eisenhart metric over the enlarged configuration space-time. In particular, it was shown that the norm $\psi = \|\boldsymbol{\xi}\|$ obeys the equation

$$\ddot{\psi} = -K_R\psi \tag{5}$$

where $K_R = \nabla^2 V(\boldsymbol{q})/N$ is the positive Ricci curvature of the manifold and V the potential of the FPU model. Supposing that the quantity K_R and the

magnitude of its fluctuations can be calculated, in the thermodynamic limit, using the Gibbs equilibrium measure and solving for the instability growth rate of Eq. (5), Casetti, Livi and Pettini [28] obtain values of the maximum Lyapunov exponent compatible with those reported in [8]. The exponent would be zero in the absence of temporal fluctuations of K_R. It is an intriguing fact that the time-periodic dependence of K_R on stable periodic (elliptic) orbits must differ enough from that on unstable periodic (hyperbolic) orbits, even if they are close in phase space, to make the Lyapunov exponent vanish. In fact, the positivity of Lyapunov exponent is caused, in this case, by the fact of being out of the spectrum of the periodic operator in (5). A more complicated case is the one of "chaotic" functions K_R. It is treated in Ref. [28] and has a close resemblance to the Anderson localization problem in one dimension.

Concerning perturbation theory results, Galgani, Giorgilli and collaborators in a recent paper [9] summarize the findings obtained using Nekhoroshev estimates [29]. The latter permit to evaluate upper bounds for the time variation of the unperturbed actions on times that, though being finite, increase exponentially as the perturbation parameter is decreased (in the FPU case the β parameter of the nonlinear term). It is possible, using this approach, to find results valid for initial conditions on open sets in the phase space, as opposed to methods based on the Kolmogorov-Arnold-Moser theorem (on the other hand the latter has the advantage to give statements valid for all times). The stability time τ of the single unperturbed actions (or action "freezing" time) is found to scale as

$$\tau = \tau_* \exp(\frac{\beta_*}{\beta})^d \tag{6}$$

where, in general, both τ_*, β_* and d depend on N. The most important dependence on N is that of d: the best estimated so far obtained for FPU gives $d \simeq N^{-1}$, a result confirmed also by numerical simulations (so the estimate seems to be optimal). This result suggests that in the thermodynamic limit the freezing times might become short, or even vanishing, and the region of violation of energy equipartition could disappear. We must, however, remember that such estimates are valid in an energy region shrinking to zero as N is increased, and moreover they are lower bounds, so they could be irrelevant. A positive result was however obtained on a modified FPU model with alternating light and heavy masses (like in a diatomic solid). In this case the harmonic frequency spectrum splits in two separated components: an "acoustic branch" with low frequencies and an "optical branch" at high frequencies; the latter is almost completely degenerate as the ratio between the masses is increased and $N \to \infty$. Then it is possible to give Nekhoroshev estimates for subsets of unperturbed actions as the total harmonic energy of the optical modes, which turns out to be frozen on a time given by the law (6), but now with $d = 1$, $\tau_* \simeq N^{-6}$ and $\beta_* \simeq N^{-8}$. Such analytical estimates suggest again the vanishing of the freezing time in the thermodynamic limit, but in this case numerical simulations show that the estimates are far from being optimal: β_* seems to be

independent of N, while τ_* has a weak dependence on N, possibly like $(\ln N)^{-1}$. The authors of Ref. [9] then argue in support of the relevance of Nekhoroshev's like estimates in the thermodynamic limit. Unfortunately, for the FPU model it is not easy to identify a natural decomposition in subsets of unperturbed actions. Perhaps this might be possible in the light of the present work, where we show the existence of subsets of normal modes where energy remains trapped for suitable initial conditions, so defining reduced (integrable or not) Hamiltonians on submanifolds of the constant energy hypersurface. It would be interesting to attempt Nekhoroshev-like estimates when the energy is restricted to these submanifolds.

More recently De Luca, Lichtenberg and Lieberman [24] studied the approach to equipartition in the FPU model exploiting normal form theory to find an effective Hamiltonian describing the interaction among a reduced number of modes (four in their treatment). The main result of their theory is that above a critical energy E_c the system reaches a near-equipartition state, in a time proportional to N^2; below this critical energy the time needed increases even faster with N (perhaps exponentially). This holds when the initial excitation is given to a subset of low modes whose number does not increase with N. If instead the excited modes are a subset scaling proportionally to N ($k \propto N$), the typical time scale to quasi-equipartition increases like N. These predictions are also supported by numerical simulations. The idea to construct the reduced Hamiltonian is to make a large N expansion of the dispertion relation $\omega_k = 2\sin[\pi k/2(N+1)] \simeq [\pi k/(N+1)] + O((k/N)^3)$ (we are treating now the system with fixed ends) and to identify the four-wave resonance relations ($k_1+k_2+k_3+k_4=0$) producing in the resonant normal form those angles which are slowly (adiabatically) varying; these latter are found to be $\theta_s = \theta_1+\theta_3-2\theta_2$ and $\theta_{sp} = \theta_2+\theta_4-2\theta_3$. The parameter controlling the deformation of the actions (monotonic in the energy) is seen to be proportional to NE, while the angles θ_s and θ_{sp} are slowly evolving with the frequency $\Omega \sim kE/N^2$; the latter determines the characteristic evolution time for the actions $\tau \sim N^2/E$ for $k \simeq$ const., while $\tau \sim N/E$ if $k \propto N$. The energy transfer to higher modes is present, but takes place on much longer times. Actually, it is also known that the energy fraction transferred to the highest modes is exponentially small in mode number [30, 31]. De Luca et al.'s idea is to use resonant normal forms and expand the dispersion relation for large N to obtain an effective Hamiltonian. This latter expansion was also suggested by Shepelyansky [32], however his purpose was to estimate the largest Lyapunov exponent which he was able to show, by his method, to be positive even at very small energies. So, according to Shepelyansky, the critical energy for the onset of chaos goes to zero as N is increased (in agreement with what is obtained in [24]). This last result is consistent with the numerical result by Pettini and Landolfi [8], but the scaling law suggested by Shepelyansky is not consistent with numerical results.

It is still difficult to arrange all these results in a single coherent framework, and especially it is not clear if it can be really justified to neglect the interaction

with high modes. In fact, we show in this paper that the structure of the interaction among the modes is rather complex.

Kantz, Livi and Ruffo [25], indipendently from De Luca et al., revealed with numerical experiments that the typical time scale for equipartition increases with N. More precisely, considering the functional dependence of the "spectral entropy" S on energy E, time t and on the number N of oscillators, these authors found that S depends only on the two variables E and t/N: $S(E,t,N) = f(E,t/N)$, for initial conditions with $k \propto N$. Moreover, for initial conditions with $k \simeq$ const. they found $S(E,t,N) = g(E/N,t/N)$. This last result is in apparent contradiction with De Luca et al., who rather seem to suggest $S(E,t,N) = g(E,t/N^2)$; but if both results have to be valid, it is clear that S must be a function of the single parameter Et/N^2. This prediction has been recently numerically confirmed [26]. Moreover, a completely independent analytical method based on the derivation of the breakdown (shock) time for the non-dispersive limit of the mKdV equation (to which the FPU-β model reduces in the continuum limit) leads to the same prediction [33]. However, a correction to this scaling theory due to a phase-space filling diffusive process is also numerically revealed [26], which finally gives a dependence of S on the single parameter $\beta Ekt/(N^2\sqrt{N})$. It should be observed that even in the thermodynamic limit at fixed E/N and with $k \propto N$, will the time scale of the system then diverge as $\sqrt{N}$. This is very intriguing because it suggests (also in the spirit of Ref. [23]) that far from equipartition states might persist in time if we perform the $N \to \infty$ limit before the $t \to \infty$ limit (a quite uncommon procedure for equilibrium statistical mechanics, but perhaps a meaningful one in non-equilibrium).

The purpose of this paper is twofold. First, we want to show several exact periodic and quasiperiodic solutions for the FPU-β system with periodic boundary conditions, whose majority appears to be new. Those which have already appeared in the literature are rederived by a unified method, which consists essentially in "extending" some harmonic modes to the anharmonic case. Second, having at our disposal explicitly known solutions, we take a first step in the study of their stability and its connection with the onset of chaos in the system. To achieve these results we rely on the structure of modal interactions in the FPU-β model, which is derived in Section 2. In Section 3 we discuss the specific fully integrable case of the three particle FPU-β model. In Section 4 we derive explicit one-mode and two-mode solutions. In Section 5 we identify two-mode and three-mode invariant submanifolds where the motion displays transitions to chaos after successive bifurcations. Section 5 is moreover devoted to a study of the restricted stability in a two-mode submanifold and to the full phase-space stability analysis of the $k = N/2$ zone-boundary solution.

2 Linear normal coordinates for the FPU-β system

Hamiltonian (1) of the FPU-β system with N particles and periodic boundary conditions can be splitted in two contributions:

$$H = H_0 + H_1 \tag{7}$$

with

$$H_0 = \frac{1}{2}\sum_{n=1}^{N} p_n^2 + \frac{1}{2}\sum_{n=1}^{N}(q_{n+1} - q_n)^2 \ , \tag{8}$$

$$H_1 = \frac{\beta}{4}\sum_{n=1}^{N}(q_{n+1} - q_n)^4 \ , \tag{9}$$

where $q_{N+1} \equiv q_1$ and $\beta > 0$.

While the interaction in physical space has the simple structure of nearest-neighbour coupling, it is clear that it becomes highly tangled when it is represented in modal (i.e. Fourier) space. Explicit expressions for the equations of motion in normal coordinates appeared sporadically in the literature for the FPU-β system in the fixed boundary case, and they were used for varied purposes. In Ref. [2] the modal equations were treated with the Krylov-Bogoliubov-Mitropolsky averaging technique, and then subjected to the criterion of overlapping resonances [34] to obtain estimates for the threshold ofstochasticity. Recently, in [24, 26] the modal equations are the starting point to develop approximations, based on normal form theory, to study the time scales to equipartition in the case when the energy is initially in a single or small group of low-frequency modes. Estimates for the FPU recurrence period were obtained by perturbative treatment of the modal equations [35]. Recently, Sholl and Henry [36] applied a shifted frequency perturbation scheme to the modal equations to perform calculations of *superperiod* recurrence times, at low anharmonicity, in FPU-α and FPU-β chains with fixed ends. In Ref. [37] the case of the FPU-β chain with fixed ends and 15 moving particles excited from rest in the 11th mode was considered (this is the most studied case were the so-called *induction period* phenomenon [38, 39] shows up); a detailed description of the early phases of the dynamics in the chain, resulting from numerical integration, was given and interpreted by means of the structure of modal couplings.

In our treatment we need to use some selection rules arising from the structure of the equations of motion in Fourier space. The first description of selection rules for the FPU-β chain with fixed ends was given by Bivins, Metropolis and Pasta [39] and later in more detail and for more general interaction potentials by Sholl [40, 41]. The case of periodic boundary conditions is slightly more involved, due to the degeneracy of the harmonic frequency spectrum, and to

our knowledge it has been given only a very brief treatment, with some missing points, in unpublished work by Sholl [41]. It is not however our purpose to give here a complete description of the selection rules arising in the periodic boundary case, which could be given along the lines of Refs. [40, 41], and we will introduce only what is strictly necessary to derive our results.

2.1 Normal coordinates for the periodic chain

Although the transformation to normal coordinates of the harmonic Hamiltonian H_0 is quite an elementary topic, it is useful to consider it in some detail to fix the notations and make some remarks.

The "unperturbed"Hamiltonian H_0 can be written, introducing the column vectors $\boldsymbol{q}$ and $\boldsymbol{p}$ of coordinates and conjugate momenta, as

$$H_0 = \frac{1}{2}\ {}^t\boldsymbol{p}\boldsymbol{p} + \frac{1}{2}\ {}^t\boldsymbol{q}\mathbf{A}\boldsymbol{q} \tag{10}$$

where ${}^t\cdot$ denotes transposition and $\mathbf{A}$ is the symmetric $N \times N$ matrix with elements

$$A_{ij} = -\delta_{i-1,j} + 2\delta_{i,j} - \delta_{i+1,j} - \delta_{i,1}\delta_{j,N} - \delta_{i,N}\delta_{j,1}\ , \qquad \begin{matrix} i = 1, \ldots, N \\ j = 1, \ldots, N \end{matrix} \tag{11}$$

Let $\mathbf{S}$ be a $N \times N$ real orthogonal (${}^t\mathbf{S}\mathbf{S} = \mathbf{I}$) matrix which makes $\mathbf{A}$ diagonal through the similarity transformation $\mathbf{A} \mapsto {}^t\mathbf{S}\mathbf{A}\mathbf{S}$. Then we can perform a canonical transformation from the old set of coordinates

$$(\ {}^t\boldsymbol{q}\,;\ {}^t\boldsymbol{p}) = (q_1, \ldots, q_N; p_1, \ldots, p_N)$$

to the new set of coordinates

$$(\ {}^t\boldsymbol{Q}\,;\ {}^t\boldsymbol{P}) = (Q_0, \ldots, Q_{N-1}; P_0, \ldots, P_{N-1})\ ,$$

by the generating function

$$F(\boldsymbol{q}, \boldsymbol{P}) = \sum_{k=0}^{N-1} \sum_{n=1}^{N} S_{nk} P_k q_n\ . \tag{12}$$

We have shifted the subscript of the new coordinates for reasons of convenience, i.e. to label the center of mass motion by the zero index. Through this transformation the harmonic part H_0 takes the form of the Hamiltonian of a system composed of $N-1$ uncoupled harmonic oscillators (the harmonic normal modes) plus a free particle (representing center of mass motion).

In view of the application of this transformation to the full anharmonic system it is important to remark that in the present case of periodic boundary conditions, owing to the degeneracy of the spectrum of $\mathbf{A}$, the matrix $\mathbf{S}$ can be

chosen in infinite different ways, leading to different sets of normal coordinates which, at variance with the harmonic case, are not equivalent for the full anharmonic Hamiltonian. Therefore the set of normal coordinates must be carefully specified.

Defining, for integer k,

$$\omega_k = 2\sin\left(\frac{\pi k}{N}\right) \ , \tag{13}$$

the eigenvalues of $\mathbf{A}$ are $\mu_k = \omega_k^2$ for $k \in \{0, 1, \ldots, [N/2]\}$[2], and they have multiplicity two, apart from μ_0 (=0) and (for even N only[3]) $\mu_{N/2}$ which are non-degenerate.

The uniquely defined (apart from a sign) normalized eigenvectors $\mathbf{u}^{(0)}$ and $\mathbf{u}^{(N/2)}$ corresponding respectively to μ_0 and $\mu_{N/2}$ have components

$$u_n^{(0)} = \frac{1}{\sqrt{N}} \ , \quad n = 1, \ldots, N \tag{14}$$

$$u_n^{(N/2)} = \frac{(-1)^n}{\sqrt{N}} \ , \quad n = 1, \ldots, N \tag{15}$$

Because of the degeneracy of the spectrum, there is freedom in the choice of an orthonormal basis in each two-dimensional eigenspace. Defining for $k = 1, \ldots, [(N-1)/2]$ the vectors $\mathbf{u}^{(k)}(\gamma)$, containing the arbitrary real parameter γ, as

$$u_n^{(k)}(\gamma) = \sqrt{\frac{2}{N}}\sin\left(\frac{2\pi k n}{N} + \gamma\right) \ , \quad n = 1, \ldots, N \tag{16}$$

it is easy to verify that

$$\mathbf{A}\mathbf{u}^{(k)}(\gamma) = \mu_k \mathbf{u}^{(k)}(\gamma) \ , \quad \forall \gamma \in \boldsymbol{R} \tag{17}$$

and that the set of N vectors $\{\mathbf{w}^{(k)}(\gamma)\}_{k\in\{0,\ldots,N-1\}}$ given by

$$\mathbf{w}^{(k)}(\gamma) = \begin{cases} \mathbf{u}^{(0)} & \text{for } k = 0 \\ \mathbf{u}^{(k)}(\gamma) & \text{for } k = 1, \ldots, [\frac{N-1}{2}] \\ \mathbf{u}^{(N/2)} & \text{for } k = N/2 \\ \mathbf{u}^{(N-k)}(\gamma + \frac{\pi}{2}) & \text{for } k = [\frac{N}{2}] + 1, \ldots, N-1 \end{cases} \tag{18}$$

is an orthonormal basis composed by eigenvectors of $\mathbf{A}$ (for each arbitrarily fixed γ). The eigenvectors corresponding to the eigenvalue μ_k ($k = 1, \ldots, [(N-1)/2]$)

[2]We denote by $[x]$ the integer part of x, so that $[N/2] = N/2$ if N is even while $[N/2] = (N-1)/2$ if N is odd.

[3]To keep generality while avoiding frequent distinctions, from now on we keep the convention that every proposition where the value $k = N/2$ appears is intended to be valid only for the even N case, while it can be simply omitted for odd N. This is true, in particular for (15) and (18).

are $\mathbf{w}^{(k)}(\gamma) \equiv \mathbf{u}^{(k)}(\gamma)$ and $\mathbf{w}^{(N-k)}(\gamma) \equiv \mathbf{u}^{(k)}(\gamma + \frac{\pi}{2})$. Once the basis, i.e. γ, is chosen, the matrix $\mathbf{S}^{(\gamma)}$ which diagonalizes $\mathbf{A}$ is given by

$$S_{nk}^{(\gamma)} = w_n^{(k)}(\gamma) \ , \qquad \begin{array}{l} n = 1, \ldots, N \\ k = 0, \ldots, N-1 \ . \end{array} \tag{19}$$

Using this matrix in the generating function of the form (12), the set of normal coordinates and momenta $(\boldsymbol{Q}^{(\gamma)}, \boldsymbol{P}^{(\gamma)})$, associated to the chosen basis, is defined by the canonical linear orthogonal transformation

$$\left\{ \begin{array}{rcl} \boldsymbol{q} & = & \mathbf{S}^{(\gamma)} \boldsymbol{Q}^{(\gamma)} \\ \boldsymbol{p} & = & \mathbf{S}^{(\gamma)} \boldsymbol{P}^{(\gamma)} \ . \end{array} \right. \tag{20}$$

For each fixed k, the set of components $\{w_n^{(k)}(\gamma)\}_{n \in \{1,\ldots,N\}}$, viewed as a function of the lattice position n, gives the spatial pattern associated to the presence of the normal coordinate $Q_k^{(\gamma)}$, since $q_n(t) = \sum_{k=0}^{N-1} Q_k^{(\gamma)}(t) w_n^{(k)}(\gamma)$. Choosing a basis amounts to a choice of the spatial phase factor γ for the stationary basis waves used to Fourier analyze the spatial pattern of the chain, given by the set $\{q_n\}$. Different basis give different Fourier components, i.e. different sets of normal coordinates. The coordinate Q_0 is proportional to the displacement of the system's center of mass, while for $k \in \{1, \ldots, [\frac{N-1}{2}]\}$ both coordinates $(Q_k^{(\gamma)}, Q_{N-k}^{(\gamma)})$ correspond, in the Fourier analysis of the spatial pattern, to the presence of a component of wavelength N/k (the lattice spacing being the unit of length) but they refer respectively to a sine and cosine wave (with respect to the chosen spatial phase). Finally the $Q_{N/2}$ coordinate corresponds to the pattern of wavelength two, where adjacent particles have equal but opposite displacements.

Every choice of the basis is equivalent *as far as the linear system is concerned* since Hamiltonian (8) takes the same form in every set of normal coordinates $(\boldsymbol{Q}^{(\gamma)}, \boldsymbol{P}^{(\gamma)})$. This is no longer true for the full nonlinear Hamiltonian H, when the same canonical transformation is applied.

2.2 Transformation of the full Hamiltonian

We now choose once for all the basis with $\gamma = \pi/4$. This is done for two reasons. Firstly, this choice simplifies the calculations since all the elements of the matrix $\mathbf{S} \equiv \mathbf{S}^{(\pi/4)}$ are given by the single expression

$$S_{nk} \equiv w_n^{(k)}(\pi/4) = \frac{1}{\sqrt{N}} \left[\sin\left(\frac{2\pi kn}{N}\right) + \cos\left(\frac{2\pi kn}{N}\right) \right] , \quad \begin{array}{l} n = 1, \ldots, N \\ k = 0, \ldots, N-1 \end{array} \tag{21}$$

Moreover, we shall see that some of the normal modes of this basis can be "extended" to the anharmonic case. From now on we denote simply $(\boldsymbol{Q}, \boldsymbol{P}) \equiv (\boldsymbol{Q}^{(\pi/4)}, \boldsymbol{P}^{(\pi/4)})$.

The quartic term H_1 in (9) is transformed into

$$H_1(\boldsymbol{Q},\boldsymbol{P}) = \frac{\beta}{4}\sum_{n=1}^{N}\left(\sum_{k=0}^{N-1}(S_{n+1,k}-S_{nk})Q_k\right)^4 \ , \tag{22}$$

with $S_{N+1,k} \equiv S_{1,k}$.

Since

$$S_{n+1,k} - S_{nk} = \sqrt{\frac{2}{N}}\,\omega_k \cos\left(\frac{\pi k(2n+1)}{N} + \frac{\pi}{4}\right) \ , \tag{23}$$

it is useful to introduce the quantities

$$U^{\delta}_{nk} \equiv \cos\left(\frac{\pi k(2n+1)}{N} + \delta\right) \ , \tag{24}$$

which obey the following rules

$$U^{\phi}_{nr}U^{\delta}_{ns} = \frac{1}{2}\left(U^{\phi+\delta}_{n,r+s} + U^{\phi-\delta}_{n,r-s}\right) \ , \tag{25}$$

$$U^{\delta+\pi}_{nr} = -U^{\delta}_{nr} \ . \tag{26}$$

The nonlinear term (22) can be rewritten in terms of these quantities as

$$H_1(\boldsymbol{Q}) = \frac{\beta}{N^2}\sum_{i,j,k,l=1}^{N-1}\omega_i\omega_j\omega_k\omega_l Q_iQ_jQ_kQ_l\sum_{n=1}^{N}U^{\pi/4}_{ni}U^{\pi/4}_{nj}U^{\pi/4}_{nk}U^{\pi/4}_{nl} \ . \tag{27}$$

Using the properties (25),(26) we get

$$\begin{aligned}\sum_{n=1}^{N}U^{\pi/4}_{ni}U^{\pi/4}_{nj}U^{\pi/4}_{nk}U^{\pi/4}_{nl} = \\ \frac{1}{8}\sum_{n=1}^{N}\left(-U^{0}_{n,i+j+k+l} + U^{0}_{n,i+j-k-l} + U^{0}_{n,i-j+k-l} + U^{0}_{n,i-j-k+l}\right) + \\ +\frac{1}{8}\sum_{n=1}^{N}\left(+U^{\pi/2}_{n,i+j+k-l} + U^{\pi/2}_{n,i+j-k+l} + U^{\pi/2}_{n,i-j+k+l} - U^{\pi/2}_{n,i-j-k-l}\right) \ .\end{aligned} \tag{28}$$

Using the identity, valid for integer r,

$$\sum_{n=1}^{N}\exp\left(i\frac{\pi r(2n+1)}{N}\right) = \begin{cases} (-1)^m N & \text{if } r = mN \text{ with } m \in \boldsymbol{Z} \\ 0 & \text{otherwise} \ , \end{cases} \tag{29}$$

we obtain

$$\sum_{n=1}^{N}U^{\pi/2}_{n,r} = 0 \quad , \forall r \in \boldsymbol{Z} \ , \tag{30}$$

and

$$\sum_{n=1}^{N} U^0_{n,r} = N\Delta_r \quad , \forall r \in \boldsymbol{Z} \ , \tag{31}$$

being

$$\Delta_r = \begin{cases} (-1)^m & \text{for } r = mN \text{ with } m \in \boldsymbol{Z} \\ 0 & \text{otherwise .} \end{cases} \tag{32}$$

From (27), (28), (30) and (31) we get

$$H_1(\boldsymbol{Q}) = \frac{\beta}{8N} \sum_{i,j,k,l=1}^{N-1} \omega_i\omega_j\omega_k\omega_l C_{ijkl} Q_i Q_j Q_k Q_l \ , \tag{33}$$

with

$$C_{ijkl} = -\Delta_{i+j+k+l} + \Delta_{i+j-k-l} + \Delta_{i-j+k-l} + \Delta_{i-j-k+l} \tag{34}$$

These integer coefficients are invariant under any permutation of the indices.

The full Hamiltonian of the FPU β-model for N oscillators with periodic boundary conditions in the new coordinates is

$$H(\boldsymbol{Q},\boldsymbol{P}) = \frac{1}{2}P_0^2 + \frac{1}{2}\sum_{i=1}^{N-1}(P_i^2 + \omega_i^2 Q_i^2) + H_1(\boldsymbol{Q}) \ . \tag{35}$$

Eliminating center of mass motion, we get easily also the equations of motion for the remaining $N-1$ degrees of freedom, which, in second order form, read

$$\begin{cases} \ddot{Q}_r &= F_r(Q_1,\ldots,Q_{N-1}) \ , \qquad r = 1,\ldots,N-1 \\ F_r(Q_1,\ldots,Q_{N-1}) &= -\omega_r^2 Q_r - \dfrac{\beta\omega_r}{2N} \displaystyle\sum_{j,k,l=1}^{N-1} \omega_j\omega_k\omega_l C_{rjkl} Q_j Q_k Q_l \ , \end{cases} \tag{36}$$

where F_r is the generalized force in normal coordinate space.

3 Intermezzo: the integrable $N = 3$ case

It is well known that the FPU β-model with $N = 3$ and periodic boundary conditions is integrable [42]. This is due to the presence of a third independent integral of motion besides energy and total momentum. In ref. [42] it is in fact shown that the quantity

$$M(\boldsymbol{q},\boldsymbol{p}) = p_1(q_2 - q_3) + p_2(q_3 - q_1) + p_3(q_1 - q_2) \tag{37}$$

is a constant of the motion. Our canonical form of the FPU Hamiltonian (33,35) allows a simple interpretation of this new integral and clarifies why it is typical of $N = 3$.

In the case $N = 3$ there are only two non-zero harmonic frequencies, the coincident pair $\omega_1 = \omega_2 = \sqrt{3}$. Invariance under permutation of indices of the C_{ijkl} coefficients in formula (33) allows to restrict the search for non zero coefficients among those with $i \geq j \geq k \geq l$. These are $C_{1,1,1,1} = C_{2,2,2,2} = 3$ and $C_{2,2,1,1} = 1$. The resulting Hamiltonian is

$$H(\boldsymbol{Q}, \boldsymbol{P}) = \frac{1}{2}P_0^2 + \frac{1}{2}\left(P_1^2 + P_2^2\right) + \frac{3}{2}\left(Q_1^2 + Q_2^2\right) + \frac{9}{8}\beta\left(Q_1^2 + Q_2^2\right)^2 \ . \qquad (38)$$

Obviously the center of mass motion is free, and P_0 is conserved. More important is the invariance of the potential term in (38) under rotations in the (Q_1, Q_2) plane, which is transparent in these new coordinates. This means that the *pseudo-angular momentum* $L = (Q_1P_2 - Q_2P_1)$ is conserved. Going back to old coordinates and momenta by the inverse of the transformation (20), we get easily the new integral in (37):

$$M = \sqrt{3}\, L \ . \qquad (39)$$

Thus, the presence of this new integral is not a surprise since it arises from a simple symmetry which was not apparent in the original coordinates; this symmetry is no more present for $N > 3$, since the potential does not have in general rotational invariance in the planes (Q_k, Q_{N-k}), but it holds true in the invariant subspace $\{N/3, 2N/3\}$ (see Subsection 4.2).

We finally observe that one can give a different interpretation of the system considered in this section. Let us think of the coordinates (q_1, q_2, q_3) as cartesian coordinates of a single particle governed by the Hamiltonian (7) with $N = 3$, thus identifying the configuration space of the three one-dimensional oscillators system with that of a single particle in three-dimensional space. The transformation to normal coordinates, being induced by an orthogonal matrix, is a rotation of the reference frame in this context, and the form (38) taken by the hamiltonian in these new coordinates reveals the cylindrical symmetry of the potential around the $\mathbf{w}^{(0)}$ axis and its independence from the Q_0 coordinate associated to the latter. From this immediately follows the conservation law for L, the angular momentum component along the $\mathbf{w}^{(0)}$ axis, and for $P_0 = (p_1+p_2+p_3)/\sqrt{3}$ which is now interpreted as the particle's momentum component $\boldsymbol{p} \cdot \mathbf{w}^{(0)}$; in fact there is no force along that direction.

We also observe that nothing changes if the quadratic part of the potential in (38) is omitted, so that also the purely quartic periodic chain with three particles is an integrable system.

4 Explicit low-dimensional solutions

From the expression (34) of the numerical coefficients appearing in the generalized force F_r in (36) it is easy to derive some selection rules already empirically

found in the literature. For instance, it is known (see e.g. [7, 31]) that for a periodic FPU-β chain with an even number of oscillators the initial excitation of a set of modes all having even (resp. odd) indices only, cannot lead to the excitation of modes having odd (resp. even) indices. This property can be easily derived observing that initial conditions of these two kinds assign a special role, among all the coefficients C_{rjkl}, to those with one index of a given parity and all the others of the opposite parity. For example, if even modes only are initially excited, it follows from (36) that odd modes can be excited only through those C_{rjkl} with only one odd index; the converse applies to the initial excitation of odd modes only. Since the algebraic sums of indices of the Δ-symbols defining the coefficients in (34) are, in both cases, always odd integers, they cannot be multiples of the even number N. Thus, all C_{rjkl} connecting (in the above sense) odd to even modes vanish.

This example shows that (for even N), if we consider the set of all modes partitioned in the two subsets of the even and odd modes, this partition has the property that an initial excitation completely contained in one of the two subsets cannot propagate to the other. It is therefore natural to wonder about the existence of other partitions of the set of modes having the same property. Exploiting this idea we are able to find some explicit periodic and quasiperiodic solutions for the FPU-β system. Though their existence, for a finite number of oscillators N, is strongly dependent on the divisibility properties of N, once the solutions are obtained and expressed in terms of the original coordinates $\{q_n\}$ they remain valid for the infinite chain.

Let us denote with $\mathcal{M}$ the set of all "internal" modes for an arbitrarily fixed number of particles N, i.e. the set of indices $\mathcal{M} \equiv \{1, \ldots, N-1\}$. The previous example leads us to introduce the following definition: a subset of modes $\mathcal{A} \subset \mathcal{M}$ is defined to be "of type I" when

$$C_{ijkl} = 0 \qquad \forall i \in \mathcal{M} \setminus \mathcal{A}\,, \quad \forall j,k,l \in \mathcal{A}\,. \tag{40}$$

It is clear that, if a subset $\mathcal{A}$ is of type I, every solution of (36) having $Q_i(0) = \dot{Q}_i(0) = 0$, $\forall i \in \mathcal{M} \setminus \mathcal{A}$, is such that $Q_i(t) \equiv 0$ $\forall t$ for the same indices i, which means that an initial excitation completely contained in $\mathcal{A}$ cannot propagate out of $\mathcal{A}$. The remaining coordinates $\{Q_j(t)\}_{j\in\mathcal{A}}$ of the solution obey a reduced system of equations of motion analogous to (36), with the only difference that the summation in the expression of the generalized force is restricted to indices $j,k,l \in \mathcal{A}$. So the normal coordinates and conjugated momenta with indices in $\mathcal{A}$ span an invariant subspace in the system's phase space, with dimension given by the double of the elements of $\mathcal{A}$; the dynamics over it is generated by the reduced Hamiltonian

$$\begin{aligned} H_{\mathcal{A}}(\{Q_j, P_j\}_{j\in\mathcal{A}}) \;&=\; \frac{1}{2}\sum_{i\in\mathcal{A}}(P_i^2 + \omega_i^2 Q_i^2) + \\ &\quad \frac{\beta}{8N}\sum_{i,j,k,l\in\mathcal{A}} \omega_i\omega_j\omega_k\omega_l C_{ijkl} Q_i Q_j Q_k Q_l\,. \end{aligned} \tag{41}$$

The subsets of even and odd modes (for even N) are just two examples of subsets of type I (each one with the additional non-generical peculiarity of having the complementary subset also of type I). It is easy to prove that these two subsets are type I independently of the chosen basis (18).

In the following subsections we discuss some low-dimensional type I subsets that we were able to identify, and their associated exact solutions. It must be remembered that we refer to the normal coordinates with $\gamma = \pi/4$ in (20).

4.1 One-mode solutions

Let us begin with the case of the simplest subsets $\mathcal{A}$: those consisting of only one mode, denoted by the index e. Then, the condition (40) for $\mathcal{A} \equiv \{e\}$ to be of type I is

$$C_{neee} = 0 \qquad \forall n \in \mathcal{M} \text{ with } n \neq e \ . \tag{42}$$

If this happens for some e, the corresponding reduced Hamiltonian (41) represents a one degree of freedom (and thus integrable) system, described by the single coordinate Q_e.

Writing the required coefficients in terms of the Δ-symbols of (32)

$$C_{neee} = -\Delta_{n+3e} + 3\Delta_{n-e} \ , \tag{43}$$

we find that for each fixed $e \in \mathcal{M}$, except for

$$e = \frac{N}{4};\ \frac{N}{3};\ \frac{N}{2};\ \frac{2N}{3};\ \frac{3N}{4} \ , \tag{44}$$

there is in $\mathcal{M}$ always one (and only one) $n \neq e$ such that $C_{neee} \neq 0$; thus condition (42) is not satisfied and $\{e\}$ is not of type I. Given a mode $e \in \mathcal{M}$ different from those listed in (44), the unique $n \in \mathcal{M}$ different from e such that $C_{neee} \neq 0$ is in fact given by the unique integer in $\mathcal{M}$ congruent to $-3e$ modulo N. Such a mode can be called the mode $n = \bar{n}(e)$ "directly forced" by mode e, since in the generalized force $F_{\bar{n}}$ in (36) a forcing term proportional to $C_{\bar{n}eee}Q_e^3$ is present. This does not mean that this mode will be the fastest growing mode, when mode e is the only one initially excited (since, of course, resonance relations must be examined), but its role is important because it acts as a trigger to excite other modes Q_j (possibly more unstable but not directly forced by mode e) through terms of the kind $C_{j\bar{n}ee}Q_{\bar{n}}Q_e^2$ in their equations of motion (36).

On the contrary, for each of the modes listed in (44) (of course when some of them exists, i.e. when N has the divisibility property required for the considered e in (44) to be an integer) property (42) is verified; thus these are the only values of e such that $\{e\}$ is a type I one-mode subset. If one of the modes in (44) is the only mode initially excited, it remains excited without transferring energy to any other mode, and the only modes that possess this property are those

in (44). In this case, the equation of motion for the excited mode amplitude Q_e is

$$\ddot{Q}_e = -\omega_e^2 Q_e - \frac{\beta \omega_e^4 C_{eeee}}{2N} Q_e^3 \ , \tag{45}$$

where C_{eeee} is always positive. The general solution of (45), having as free parameters the amplitude A and the time origin t_0, is

$$Q_e(t) = A \, \mathrm{cn} \left[\Omega_e (t - t_0) \, , \, k \right] \ , \tag{46}$$

where Ω_e and the modulus k of Jacobi elliptic cosine function[4] both depend on A:

$$\Omega_e = \omega_e \sqrt{1 + \delta_e A^2} \tag{47}$$

$$k = \sqrt{\frac{\delta_e A^2}{2(1 + \delta_e A^2)}} \ , \tag{48}$$

with $\delta_e = \beta \omega_e^2 C_{eeee}/(2N)$. We remind that this solution is periodic, with amplitude dependent period T_e given in terms of the complete elliptic integral of the first kind $K(k)$ by

$$T_e = \frac{4K(k)}{\Omega_e} \ . \tag{49}$$

Since A is one-to-one related to the control parameter (3) involving the energy density, all parameters of the solution (46) can be rewritten as functions of ϵ instead of A. For the period we have

$$T_e = \frac{4K(k)}{\omega_e (1 + 2\epsilon C_{eeee})^{1/4}} \ , \tag{50}$$

where $k = k(\epsilon)$. The period decreases as ϵ is increased, while in the limit $\epsilon \to 0$ it reduces to the harmonic period $T_e \to 2\pi/\omega_e$.

All one-mode solutions correspond to stationary waves of the form

$$q_n(t) = Q_e(t) w_n^{(e)} \tag{51}$$

where the vectors $\mathbf{w}^{(e)} \equiv \mathbf{w}^{(e)}(\pi/4)$ are given in formula (21). The spatial pattern is therefore the same of the corresponding linear mode, but these are *nonlinear modes* since the time dependence corresponds to a nonlinear oscillation, which reduces to the usual harmonic one as A goes to zero.

Let us first discuss the lattice pattern of the solution corresponding to $e = N/2$, i.e. its expression as a function of the old set of coordinates:

$$q_n(t) = \frac{(-1)^n}{\sqrt{N}} Q_{N/2}(t) \ , \tag{52}$$

[4]For standard notation and properties of elliptic functions and integrals we refer to [43, 44].

where $Q_{N/2}(t)$ is given by Eqs. (46), (47) and (48), with $e = N/2$, $\omega_{N/2} = 2$, $\delta_{N/2} = 4\beta/N$. The lattice pattern has adjacent particles with opposite phases, being the same of the zone-boundary phonon mode. Actually, this solution is present for any potential of the form

$$V = \sum_{n=1}^{N} \Phi(q_{n+1} - q_n) \ . \tag{53}$$

with even N on a periodic lattice (or on an infinite lattice). In fact, after the substitution of the ansatz solution $q_n = (-1)^n r(t)$, the equations of motion reduce to the single equation for $r(t)$

$$\ddot{r} = -2\frac{d\Phi_{even}}{dr}(2r) \ , \tag{54}$$

where $\Phi_{even}(r) \equiv (\Phi(r) + \Phi(-r))/2$ is the even part of the Φ function. For instance, a solution of this kind is known for the integrable case of the Toda lattice and corresponds to the standing cnoidal wave with two lattice spacings wavelength [45].

The cases $e = N/4$ and $e = 3N/4$ are treated in a similar way. The lattice pattern is

$$q_n(t) = \frac{1}{\sqrt{N}}\, Q_e(t) \left[\pm \sin\left(\frac{\pi n}{2}\right) + \cos\left(\frac{\pi n}{2}\right) \right] \tag{55}$$

where $Q_e(t)$ is given by Eqs. (46), (47) and (48) with $\omega_{N/4} = \omega_{3N/4} = \sqrt{2}$, $\delta_{N/4} = \delta_{3N/4} = 4\beta/N$, and the '$+$' and '$-$' signs correspond to $e = N/4$ and $e = 3N/4$ respectively. Let us observe that the solution $e = 3N/4$ is obtained from that with $e = N/4$ by shifting the lattice pattern by one lattice spacing; another shift produces the same solution apart from a temporal phase. This property is a consequence of the invariance of the model under translations of an integer number of lattice spacings.

Because of an additional peculiarity, the single mode solutions $e = N/3$ and $e = 2N/3$ will be treated in the following as particular cases of the two-mode manifolds.

4.2 Two-mode manifolds

We do not try here to identify all multi-mode, or even two-mode, type I subsets for generic N, although some of them can be found by simple inspection of a computed table of non-zero C_{ijkl} coefficients[5] for small N. Instead we confine ourselves to the search of two-mode type I subsets of the kind $\{i, N-i\}$, since in this case we get complete results leading to periodic and quasiperiodic explicit solutions.

[5]For example, it can be seen that $\{1,5\}$ and $\{3,7\}$ for $N = 8$, or $\{1,5,9\}, \{2,6,10\}$ and $\{3,7,11\}$ for $N = 12$ are all of type I.

A subset $\{i, N-i\}$ is of type I when (see condition (40))

$$C_{njkl} = 0 \qquad \forall n \in \mathcal{M} \setminus \{i, N-i\},\ \forall j,k,l \in \{i, N-i\}\ . \tag{56}$$

Thus, in particular, a *necessary* condition is

$$C_{niii} = 0 \qquad \forall n \in \mathcal{M} \text{ with } n \neq i, N-i\ . \tag{57}$$

This can happen, *a priori*, only in two cases: *a)* $\{i\}$ is of type I, or *b)* $\{i\}$ is not type I but the mode $\bar{n}(i)$, directly excited by i, is coincident with $N-i$. But it is easy to see, from the explicit expression of $\bar{n}(i)$, that case *b)* can never happen: then if i is such that $\{i, N-i\}$ is of type I, it must be one of the modes in (44). The only subsets of the kind requested that can be type I are therefore $\mathcal{E}_1 \equiv \{N/4, 3N/4\}$ and $\mathcal{E}_2 \equiv \{N/3, 2N/3\}$. To check that they are indeed, it is useful to remark that

$$C_{N-i,\,N-j,\,N-k,\,N-l} = C_{ijkl}\ . \tag{58}$$

Then, since i verifies (42) with $e = i$ (and also $N-i$ does), from (58) we need only to check that

$$C_{n,\,i,\,i,\,N-i} = 0 \quad \forall n \in \mathcal{M} \setminus \{i, N-i\} \tag{59}$$

for condition (56) to be satisfied.

Let us first consider the set $\mathcal{E}_1$. Using formula (34) we have

$$C_{n,\,N/4,\,N/4,\,3N/4} = -\Delta_{n+5N/4} + 2\Delta_{n-3N/4} + \Delta_{n+N/4}\ , \tag{60}$$

and each Δ-symbol vanishes for $n \notin \mathcal{E}_1$, thus satisfying (59). This proves that the set $\mathcal{E}_1$ is of type I, i.e. the excitation of the the pair $\{N/4, 3N/4\}$ does not propagate to other modes. Moreover, Hamiltonian (41) with $\mathcal{A} = \mathcal{E}_1$, describing the reduced system containing only this pair of modes, is separable because the coefficients (60) are zero also for $n \in \mathcal{E}_1$, giving

$$H_{\mathcal{E}_1} = \frac{1}{2}\left(P_{N/4}^2 + P_{3N/4}^2\right) + Q_{N/4}^2 + Q_{3N/4}^2 + \frac{2\beta}{N}\left(Q_{N/4}^4 + Q_{3N/4}^4\right) \tag{61}$$

Being separable, this Hamiltonian is integrable. Thus, the motion in the subspace of the modes $\{N/4, 3N/4\}$ is simply given by the cartesian product of the one-mode solutions already introduced in the previous subsection. However, it is interesting to observe that this two-mode invariant manifold foliated in two-dimensional tori exists in the $2N$-dimensional phase space of the system, with periodic or quasiperiodic trajectories whose winding number depends on the non-linear periods of the two modes (see formula (49)). Therefore we are able to obtain quasiperiodic solutions with two frequencies exploiting the fact that anharmonicity, causing the nonlinear dependence on amplitude of the period (49),

"removes" the harmonic frequency degeneracy of the pair $\{N/4, 3N/4\}$. The general solution (see formula (46)) is

$$
\begin{aligned}
q_n(t) = & \qquad (62)\\
& \frac{1}{\sqrt{N}} A_{N/4}\, \mathrm{cn}\left[\Omega_{N/4}(A_{N/4})\, t + \phi,\, k(A_{N/4})\right] \left[\sin\left(\frac{\pi}{2}n\right) + \cos\left(\frac{\pi}{2}n\right)\right] + \\
& \frac{1}{\sqrt{N}} A_{3N/4}\, \mathrm{cn}\left[\Omega_{3N/4}(A_{3N/4})\, t + \psi,\, k(A_{3N/4})\right] \left[-\sin\left(\frac{\pi}{2}n\right) + \cos\left(\frac{\pi}{2}n\right)\right] \ ,
\end{aligned}
$$

where we have emphasized the dependence of the various parameters on the two independent arbitrary amplitudes $A_{N/4}$ and $A_{3N/4}$. It is interesting to observe that

$$q_{n+2} = -q_n \ , \qquad (63)$$

which explains why a mode with a wavelength of four lattice sites corresponds to a solution with two degrees of freedom. When the amplitudes of the two modes in (62) are equal (we omit in this case the moduli in the arguments of the cn functions since they are equal) one gets periodic solutions. In particular, for the two choices of the phase difference $\psi - \phi = 0$ and $\psi - \phi = 2K$, stationary wave solutions are obtained. They correspond to a lattice pattern having one node every two lattice sites, thus giving also a solution valid for fixed end chains, after an appropriate choice of the lattice origin. It should also be observed that these latter would be one-mode solutions in the normal coordinates relative to the basis (18) with $\gamma = 0$.

If instead we choose $\psi - \phi = \pm K$ [still with equal amplitudes, denoted by A, and with $K \equiv K(k(A))$] the corresponding periodic solutions have the property

$$q_{n+1}(t \pm \Delta t) = q_n(t) \ , \quad \text{for } \Delta t = K/\Omega_{N/4}(A) \ , \forall n \ , \qquad (64)$$

where the sign in the argument in the l.h.s. is the same of $(\psi - \phi)$. We consider (64) as the defining property of a travelling wave on a lattice, propagating respectively to the right ('+' sign) or to the left ('−' sign) with velocity $1/\Delta t$ (the lattice spacing being the unit of length). We remark that the velocity depends on the amplitude, as should be expected for a nonlinear wave. Actually, observing that, for integer n, the following identities hold

$$
\begin{aligned}
\sin\left(\frac{\pi}{2}n\right) \mathrm{cn}(x) &= \frac{1}{2}\left\{\mathrm{cn}[K(n-1)+x] + \mathrm{cn}[K(n-1)-x]\right\} \ , \qquad (65)\\
\cos\left(\frac{\pi}{2}n\right) \mathrm{cn}(x) &= \frac{1}{2}\left\{\mathrm{cn}(Kn+x) + \mathrm{cn}(Kn-x)\right\} \ , \qquad (66)
\end{aligned}
$$

and defining the function

$$\mathrm{g}(x,k) \equiv \mathrm{cn}(x - K(k),\, k) + \mathrm{cn}(x,k) \ ,$$

it is straightforward to rewrite the general solution (62), for excitations in the $\mathcal{E}_1$ subspace, in a form which reveals its progressive and regressive travelling

wave content, in analogy with the harmonic case:

$$q_n(t) = \frac{1}{2\sqrt{N}}\left[A_a \mathrm{g}(K_a n + \Omega_a t + \phi,\, k_a) + A_b \mathrm{g}(K_b(n+1) + \Omega_b t + \psi,\, k_b)\right] + \frac{1}{2\sqrt{N}}\left[A_a \mathrm{g}(K_a n - \Omega_a t - \phi,\, k_a) + A_b \mathrm{g}(K_b(n+1) - \Omega_b t - \psi,\, k_b)\right] \ . \tag{67}$$

In (67) we have denoted the quantities relative to the modes $N/4$ and $3N/4$ by the indices 'a' and 'b' respectively. The particular cases above, with $A_a = A_b = A$ and $\psi - \phi = \pm K$ are

$$q_n(t) = \frac{A}{\sqrt{N}}\,\mathrm{g}\left(Kn \mp \Omega_{N/4}(A)\, t \mp \phi\right) \ , \tag{68}$$

where we have made explicit the travelling wave nature of these solutions.

Turning now to the other set $\mathcal{E}_2$, we have

$$C_{n,\,N/3,\,N/3,\,2N/3} = -\Delta_{n+4N/3} + 2\Delta_{n-2N/3} + \Delta_n \ , \tag{69}$$

and again we find that all Δ's vanish for $n \notin \mathcal{E}_2$, thus proving that also $\mathcal{E}_2$ is of type I. This time there is a non-zero case among the different kinds of coefficients coupling the two modes of this subset, e.g. $C_{N/3,\,N/3,\,2N/3,\,2N/3} = 1$, and the reduced Hamiltonian is

$$H_{\mathcal{E}_2} = \frac{1}{2}\left(P_{N/3}^2 + P_{2N/3}^2\right) + \frac{3}{2}\left(Q_{N/3}^2 + Q_{2N/3}^2\right) + \frac{27\beta}{8N}\left(Q_{N/3}^2 + Q_{2N/3}^2\right)^2 \ . \tag{70}$$

Let us first remark that this Hamiltonian reduces to the one of formula (38) for $N = 3$ apart from the center of mass motion term, which has already been eliminated. Being the potential in (70) invariant under rotation in the $(Q_{N/3}, Q_{2N/3})$ plane, again, as for the $N = 3$ case, the "angular momentum" $(Q_{N/3}P_{2N/3} - Q_{2N/3}P_{N/3})$ is conserved. Thus, having two constants of motion in involution, Hamiltonian (70) is integrable. We have again an invariant manifold foliated by two-dimensional tori, but the explicit general solution for Hamiltonian (70), although possible in principle, is less trivial in this case. However, we can easily find some lower dimensional solutions. In fact, the presence of a central potential implies that there exist solutions whose trajectory on the $(Q_{N/3}, Q_{2N/3})$ plane is an oscillation lying on an arbitrary chosen straight line crossing the origin. Hence, this implies that not only the modes $N/3$ and $2N/3$ are particular one-mode solutions, as we have already anticipated, but that there are analogous solutions corresponding to all possible choices (rotations) of the basis (18); this property is not present for the set $\mathcal{E}_1$. Each one of these solutions with zero "angular momentum" would be regarded as one-mode if we had chosen a linear basis with the convenient value of γ in formula (18). In the original lattice coordinates $\{q_n\}$ they are stationary waves, with a pattern given

by an arbitrary continuous translation of the stationary sine wave of wavelength three. All these one-mode solutions satisfy the same differential equation (45), with $\omega_e = \omega_{N/3} = \sqrt{3}$ and $C_{eeee} = C_{N/3,\,N/3,\,N/3,\,N/3} = 3$. The lattice pattern is

$$q_n(t) = \sqrt{\frac{2}{N}}\, A\,\mathrm{cn}\left[\Omega_{N/3}(t-t_0),\, k\right] \sin\left(\frac{2\pi}{3}n + \gamma\right)\ , \tag{71}$$

where γ is an arbitrary real parameter; $\Omega_{N/3}$ and k are given by (47) and (48) with $\delta_e = \delta_{N/3} = 9\beta/(2N)$. It is interesting to observe that for a generic value of γ this solution has no nodes (still oscillators) at lattice sites. The only case in which nodes appear is $\gamma = 0$ (the cases $\gamma = \pi/3$ and $\gamma = 2\pi/3$ can be reduced to this one after a translation of a lattice unit), and it is clearly present also for fixed ends oscillator chains.

Also for the set $\mathcal{E}_2$ travelling wave solutions exist. They correspond to closed orbits for the central potential in Hamiltonian (70). A particularly simple case is the one of closed circular orbits:

$$\begin{cases} Q_{N/3}(t) &= A\cos\left[\Omega_{N/3}(t-t_0)\right] \\ Q_{2N/3} &= \pm A\sin\left[\Omega_{N/3}(t-t_0)\right]\ . \end{cases} \tag{72}$$

The lattice pattern is

$$q_n(t) = \sqrt{\frac{2}{N}}\, A\,\sin\left(\frac{2\pi}{3}n \pm \Omega_{N/3}\, t + \phi\right) \tag{73}$$

where ϕ is an arbitrary phase. This solution is of the form of the linear travelling wave, but has amplitude dependent frequency and velocity, since $\Omega_{N/3} = \Omega_{N/3}(A)$.

Finally, we further stress that, though for the FPU-β system with finite N each of these solutions exists only for suitable (but still infinitely many) values of N, their expressions in terms of the original $\{q_n\}$ coordinates remain valid as spatially periodic solutions for the infinite chain. The "out-of-phase" oscillation (52) and the one-mode $N/4$ solution with $\gamma = 0$ (given by our solution (62) in the particular case $A_{N/4} = A_{3N/4}$, $\psi = \phi$) appeared first in [46], where they were obtained directly in particle displacement coordinates by a suitable "ansatz". A statement equivalent, in our notation, to the fact that an excitation in the subsets $\mathcal{E}_1$ or $\mathcal{E}_2$ cannot propagate out of these sets, was given in unpublished work by Sholl [41].

5 Stability of periodic orbits

In the previous Section we have shown the existence, in the phase space of the FPU-β system, of various kinds of initial conditions giving rise to trajectories lying on manifolds of smaller dimension than that of the constant energy shell.

We have considered in detail some simple cases leading to reduced integrable systems, thus obtaining some families of explicit solutions. In our opinion these are interesting in their own, since explicit analytical solutions, are not common at all for nonlinear *non-integrable* chains of oscillators. However we must remember that all these results hold for *particular* classes of initial conditions. Therefore an important problem is that of the stability of these solutions or, more generally, of these invariant subspaces. If one of them turns out to be stable, then its qualitative features are present for a non-zero measure neighbourhood of initial conditions in phase space, thus acquiring physical significance.

From another point of view, it is reasonable to expect some relation between loss of stability of periodic orbits (or more generally of invariant subspaces) and the onset of chaos in the system. This is suggested by the generic behaviour of near-integrable Hamiltonian systems where, as the perturbation parameter is increased, the "chaotic sea" expands in phase space, forcing regular regions to shrink. Budinsky and Bountis [46], conjectured that the destabilization of known periodic orbits of an Hamiltonian system, although being only a local property, could give an upper bound estimate for the onset of large-scale chaos. This suggestion was perhaps not fully justified since, at that time, only few one-mode solutions (e.g. $e = N/2$) were known, and moreover the behaviour of very low-dimensional systems (e.g. Hénon-Heiles) had been studied. It assumes more relevance now, since we know that several invariant manifolds exists. However, the fact that periodic and quasiperiodic solutions lose stability or invariant submanifolds become unstable does not necessarily imply large-scale chaos. We will show that this loss of stability leads to the formation of stochastic layers, but their thickness and extension in phase space remain small at small ϵ. In modal space, the instability of all these newly discovered submanifolds does not lead to energy equipartition if ϵ is sufficiently small, but to exponentially localized mode energy spectra with irregular, chaotic, time dependencies of mode energies.

5.1 Bifurcation and transition to chaos in a reduced system

It is easy to verify that the set $\mathcal{F} = \{N/4, N/2, 3N/4\}$ is of type I. Again, one has to verify condition (40) for $\mathcal{A} = \mathcal{F}$. Apart from permutations of the indices, there are ten distinct kinds of coefficients to consider, corresponding to the number of triplets that can be formed with the elements of $\mathcal{F}$ without regard to order and with allowed repetition of any element. Five of them belong to cases already treated in Secs. 4.1 and 4.2. Examining also the remaining cases, we find that the only non-zero coefficients having three indices in $\mathcal{F}$ and the remaining index *unrestricted* (in $\mathcal{M}$) are, apart from permutations, $C_{N/4,\,N/4,\,N/2,\,N/2} = C_{3N/4,\,3N/4,\,N/2,\,N/2} = 2$ and, of course, the three C_{eeee} with $e \in \mathcal{F}$. This allows to conclude that $\mathcal{F}$ is of type I, and at the same time

leads to write the corresponding reduced Hamiltonian:

$$H_{\mathcal{F}} = \frac{1}{2}\left(P_{N/4}^2 + P_{N/2}^2 + P_{3N/4}^2\right) + Q_{N/4}^2 + 2Q_{N/2}^2 + Q_{3N/4}^2 + \frac{2\beta}{N}\left(Q_{N/4}^4 + 2Q_{N/2}^4 + Q_{3N/4}^4 + 6Q_{N/4}^2 Q_{N/2}^2 + 6Q_{3N/4}^2 Q_{N/2}^2\right). \quad (74)$$

Either from the corresponding equations of motion, or from what has been found above concerning the coefficients, we observe that there exist also two new two-mode invariant subspaces: that of the pair $\{N/4, N/2\}$ and that of $\{3N/4, N/2\}$. At variance with cases discussed in Secs. 4.1–4.2, all these new invariant sets give rise to seemingly non-integrable Hamiltonians. The case of a two-mode invariant subset is particularly interesting because, for such a reduced system, the qualitative features of the dynamics can be visualized on a two-dimensional Poincaré section.

The equations of motion corresponding to the set $\{N/4, N/2\}$ are:

$$\begin{cases} \ddot{Q}_{N/4} = -2Q_{N/4} - 8\dfrac{\beta}{N}Q_{N/4}^3 - 24\dfrac{\beta}{N}Q_{N/4}Q_{N/2}^2 \\ \ddot{Q}_{N/2} = -4Q_{N/2} - 16\dfrac{\beta}{N}Q_{N/2}^3 - 24\dfrac{\beta}{N}Q_{N/2}Q_{N/4}^2 \, . \end{cases} \quad (75)$$

Those relative to the other set $\{3N/4, N/2\}$ are identical, substituting $Q_{N/4} \to Q_{3N/4}$. Rescaling the coordinates by $\sqrt{\beta/N}$ one obtains equations independent of the ratio β/N. Thus an orbit of the system (75) is mapped to one of the same system with $\beta/N = 1$. This means that the system (75) remains meaningful in the termodynamic limit.

We want, in particular, to investigate the stability of the "out-of-phase" nonlinear oscillation (52), i.e. the one-mode periodic solution (46) having $e = N/2$. Therefore we choose the $(Q_{N/4}, P_{N/4})$ plane as the surface of section; in fact on this plane that solution is represented by a fixed point for the Poincaré first return map, located at $(Q_{N/4}, P_{N/4}) = (0, 0)$. The one-mode solution with $e = N/4$ lies, instead, on the surface of section and can be drawn simply as the curve bounding the energetically accessible region. In Figs. 1, 2 and 3 we show numerically generated Poincaré sections for the system (75), corresponding to three different increasing values of the control parameter ϵ in (3). For each ϵ value, the intersections originated by several different initial conditions are shown, together with the bounding curve corresponding to mode $e = N/4$.

We observe that the fixed point at the origin is stable at low values of ϵ. When the energy density is increased, a bifurcation occurs, giving rise to a pair of stable fixed points, while the original one loses stability. A small closed invariant curve which surrounds only one of them is plotted in Fig. 2 to make clear the presence of two distinct fixed points (i.e. two different bifurcated orbits for the flow), so that the bifurcation is not period-doubling. To confirm this we have also numerically computed the eigenvalues (Λ_1, Λ_2) of the Poincaré map

linearized around the origin, obtaining a more precise estimation of the critical ϵ value. As ϵ is increased the eigenvalues, lying on the unit circle in the complex plane, move on it until they collide at $\Lambda_1 = \Lambda_2 = +1$ for $\epsilon = 1.127$ and then move apart on the real axis. After the fixed point at the origin turns unstable, a stochastic layer is originated by homoclinic intersections, too thin to be seen in Fig. 2 but already very thick in Fig. 3. Therefore when the stationary wave (52) has high enough amplitude and is perturbed only by a small component along mode $N/4$, the interaction between the two modes leads to chaotic behaviour. However even at the ϵ value of Fig. 3 we do not observe transport over the full phase space which is signature of large-scale chaos (which, of course, will set in at larger values of ϵ). This shows that the loss of stability of periodic orbits induces the appearence of stochastic layers but the large-scale chaos phenomenon is not a direct consequence of it, contrary to the expectations of Ref. [46].

In the next Subsection we study the stability problem for the $e = N/2$ mode in the full phase space.

5.2 Large N stability

The problem of stability of a known solution $\overline{\boldsymbol{Q}}(t)$ under generic small perturbations in the initial data, is tackled by studying the variational equations, obtained by linearizing system (36) around $\overline{\boldsymbol{Q}}(t)$. Let $\boldsymbol{x}(t) = \boldsymbol{Q}(t) - \overline{\boldsymbol{Q}}(t)$ be the small separation vector between a solution $\boldsymbol{Q}(t)$, initially close to $\overline{\boldsymbol{Q}}$, and the reference solution $\overline{\boldsymbol{Q}}(t)$ itself. Then $\boldsymbol{x}$ obey, in linear approximation, the following system of equations:

$$\ddot{x}_r = \sum_{s=1}^{N-1} B_{rs}(t) x_s, \qquad r = 1, \ldots, N-1 \ , \tag{76}$$

where

$$B_{rs}(t) = \left. \frac{\partial F_r}{\partial Q_s} \right|_{\boldsymbol{Q}=\overline{\boldsymbol{Q}}(t)} . \tag{77}$$

is the Jacobian matrix of $\boldsymbol{F}$ evaluated on the reference solution. We limit ourselves to study here the stability of the periodic single-mode $\{e\}$ solutions $\overline{Q}_j(t) = \delta_{je} Q_e(t)$, with $Q_e(t)$ given by (46). In this case system (76) reduce to

$$\ddot{x}_r = -\omega_r^2 x_r - \frac{3\beta}{2N} \omega_r \omega_e^2 Q_e^2(t) \sum_{s=1}^{N-1} \omega_s C_{rs}^{(e)} \, x_s \ , \qquad r = 1, \ldots, N-1 \tag{78}$$

where the coupling matrix, which depends on the chosen mode e in (44), has elements $C_{rs}^{(e)} \equiv C_{rsee}$. It turns out that $C_{rs}^{(e)}$ is diagonal only for $e = N/2$, with $C_{rs}^{(N/2)} = 2\delta_{rs}$. The study of the stability of the $e = N/2$ nonlinear mode is therefore simpler, because the different components of the perturbation in modal space are all decoupled and can be studied separately, each one being

a problem of parametric excitation described by an equation of the Hill type. This permits approximate semi-analytic estimates also for what concerns the dependence of stability properties on the number N of oscillators. Accordingly, we restrict here to the case $e = N/2$. The study of other one-mode cases (e.g. $e = N/3$) would imply the study of the stability for a system of coupled linear equations with periodic coefficients, a more complex problem of many degrees of freedom parametric excitation. This could be done by producing numerically the appropriate transfer matrix, but such a procedure should be repeated for each fixed value of N and the large N result should be extrapolated.

For $e = N/2$, after using (46), Eqs. (78) reduce to a set of decoupled Lamé equations [47, 48]

$$\ddot{x}_r = -\omega_r^2 \left[1 + 12 \frac{\beta A^2}{N} \mathrm{cn}^2(\Omega_{N/2} t, k) \right] x_r \ , \qquad r = 1, \ldots, N-1 \ , \tag{79}$$

with $\Omega_{N/2}$ and k depending on A as given in (47) and (48). The physical control parameter, proportional to the energy density, is ϵ, which is in a one-to-one relation with A. However the analysis is simpler if we choose the modulus k as a control parameter. In fact, as ϵ is varied from zero to $+\infty$, the modulus k increases monotonically in the interval $[0, 1/\sqrt{2}\,)$, the limit $\epsilon \to +\infty$ corresponding to $k \to 1/\sqrt{2}$. The relation $\epsilon(k)$ is

$$\epsilon = \frac{k^2}{1-2k^2} \left(1 + \frac{k^2}{1-2k^2} \right) \ . \tag{80}$$

Expressing $\Omega_{N/2}$ and $\beta A^2/N$ as functions of k, and after rescaling time at each fixed k (which does not alter stability properties), each of the equations in (79) can be put in the standard Jacobian form of Lamé equation [47, 48]

$$y'' + [\alpha - \nu(\nu+1) k^2 \mathrm{sn}^2(u, k)]\, y = 0 \ , \tag{81}$$

where the prime superscript denotes differentiation with respect to the new time $u = \Omega_{N/2} t$ and y stands for the generic variable x_r. For the perturbation component x_r in the direction of mode number r, the parameters in (81) are

$$\alpha = (1 + 4k^2)\omega_r^2/4 \ ; \quad \nu(\nu+1) = 3\omega_r^2/2 \ . \tag{82}$$

We observe that dependence on the mode number r and on the number N of oscillators comes only through the ratio r/N appearing in ω_r (see eq. (13)). This allows to discuss in an unified way also the dependence on the system size N. In fact, we can fix ϵ and then consider two systems of different sizes N_1 and N_2; the linearized equations for a mode r_1 in system N_1 and for a mode r_2 in system N_2 are the same if $r_1/N_1 = r_2/N_2$.

Resuming, we discuss the stability of the zero solution of (81) as a function of two parameters (ρ, k) with $0 \le \rho < 1$, $0 \le k < 1/\sqrt{2}$, when (α, ν) are given by

$$\alpha = \rho(1 + 4k^2) \ ; \quad \nu(\nu+1) = 6\rho \ . \tag{83}$$

A given pair (ρ, k) describes at the same time different mode numbers r in systems with different N, all having the same r/N value given by the relation $\rho = \sin^2(\pi r/N)$, with the same ϵ for the unperturbed solution $e = N/2$. We first consider ρ as a continuous parameter, which corresponds to the limit $N \to \infty$, and then we discuss what happens when ρ can take only a finite set of values, as it is for any finite N.

For integer ν many rigorous results are known for eq. (81) [47, 48], and it is in particular known [49] that there are only $\nu + 1$ instability regions in the (α, k) plane. However, in our case only the integer values $\nu = 1$ and $\nu = 2$ are possible, corresponding to $\rho = 1/3$ and $\rho = 1$, respectively. The stability charts in the (α, k) plane for these two integer ν cases of eq. (81) have been explicitly constructed in [50]. The second case $\rho = 1$, is of limited interest to us since it corresponds to $r = N/2$, i.e. to perturbations along the invariant subspace $e = N/2$; the results in [50] just confirm that there exists a periodic solution for $x_{N/2}$ at all k values, as it must a priori be, since it corresponds to a perturbation along the periodic orbit $Q_{N/2}(t)$ under study. More interesting is the case $\rho = 1/3$: the representative point in the (α, k) parameter plane of (81) with $\nu = 1$ moves on the curve $\alpha = (1 + 4k^2)/3$ as k is varied, and we find (see Fig. 4 of Ref. [50]) that it lies always in the first stable region for $0 \leq k < 1/\sqrt{2}$. It touches the boundary curve of the instability tongue only for $k = 1/2$. Therefore the mode corresponding to $\rho = 1/3$ is stable (as a perturbation to $e = N/2$) at any finite energy density ϵ, and reaches the stability border only asymptotically for $\epsilon \to \infty$.

To solve the stability problem in the generic ν case we approximately reduce eq. (81) to Mathieu equation, whose stability diagram is well known [44, 48]. In fact, in the parameter region of our interest $0 < k^2 < 1/2$, the function sn^2 appearing in (81) is well approximated by its first order Fourier development. This latter is given by

$$k^2 \mathrm{sn}^2(u, k) = 1 - \frac{E}{K} - \left(\frac{\pi}{K}\right)^2 \sum_{n=1}^{\infty} \frac{n}{\sinh(n\pi K'/K)} \cos\left(\frac{n\pi u}{K}\right) \ , \qquad (84)$$

where K and E are the complete elliptic integrals of first and second kind, respectively, with modulus k, while $K'(k) = K(\sqrt{1 - k^2})$. The Fourier coefficients are exponentially decreasing with order n, the more rapidly the smaller k is. In the worst case to consider, i.e. $k \to 1/\sqrt{2}$ the ratio between the $n = 2$ and $n = 1$ coefficients is ≈ 0.086. Furthermore, we are interested in the modes which first go unstable, i.e. which possibly destabilize at small k, and for them the error is much smaller. Therefore, we truncate (84) keeping only the $n = 1$ term and obtain, after a further time rescaling $\tau = \pi u/2K$, the canonical form of Mathieu equation:

$$\frac{d^2 y}{d\tau^2} + [a - 2q\cos(2\tau)]\, y = 0 \ , \qquad (85)$$

where

$$a = \rho \left(\frac{2K}{\pi}\right)^2 \left(-5 + 4k^2 + 6\frac{E}{K}\right) \;\; ; \quad q = -\frac{12\rho}{\sinh(\pi K'/K)} \; . \tag{86}$$

Both parameters a and q depend on k^2 and ρ, therefore for each fixed ρ (which corresponds to fix a ratio r/N), changing k^2 (and correspondingly the energy density ϵ) amounts to trace a curve in the (q, a) parameter plane. A stability transition happens if this curve intersects characteristic curves separating stable from unstable regions for the Mathieu equation. In our case intersections can occur only with the characteristic curve $b_1(q)$ (we use the standard notation, see e.g. [44]) bounding from below the first tongue of instability. In Fig. 4 we show the (q, a) curves (86) at fixed ρ and varying k for positive[6] q, and those at fixed k and varying ρ, together with the characteristic curves $b_1(q)$ and $a_1(q)$ bounding the first instability tongue. This mesh provides a reference frame to locate the values of ρ and k corresponding to stable or unstable cases. We do not trace the $\rho = 1$ curve which superposes with $a_1(q)$, showing only a slight deviation for $k^2 > 0.4$. This superposition is expected because the truncation to the first Fourier coefficients in (84) only slightly affect the exact solution of the Lamé equation in the $\nu = 1$ case. We see that curves with fixed ρ enter the instability region, for some critical value $k_c(\rho)$ of k, only for ρ larger than a value such that the corresponding curve touches $b_1(q)$ only asymptotically for $k \to \infty$. We numerically find such a value to be $\rho \simeq 0.33$, which therefore must be identified with the value $\rho = 1/3$ having rigorously this property for the exact Lamé equation, as seen before. This confirms the accuracy of the Mathieu approximation. Also, we find that the $\rho = 1/2$ ($r = N/4$) curve intersects b_1 for $\epsilon \simeq 1.13$, in excellent agreement with the value $\epsilon = 1.127$ for the instability threshold in the $r = N/4$ direction, obtained from the Poincaré map in Subsection 5.1.

We have computed, for several values of $\rho > 1/3$, the critical $k_c(\rho)$ value at which the corresponding constant ρ curve intersects the b_1 line. Returning to the physical control parameter ϵ by (80) we finally construct the marginal stability curve $\epsilon_c(\rho)$ in Fig. 5. Now we remember that, for a given number N of oscillators, only the discrete set of ρ values

$$\rho = \sin^2(\pi r/N) \; , \qquad r = 1, \ldots, N-1 \tag{87}$$

must be considered. From Fig. 5 we see that for each mode having $\rho > 1/3$ there is a threshold value $\epsilon_c(\rho) \neq 0$ for instability. Above $\epsilon_c(\rho)$ the $e = N/2$ nonlinear mode develops an instability causing growth of the mode corresponding to ρ through parametric resonance. On the contrary, modes with $\rho < 1/3$ (i.e. $r/N < 0.196$) are always stable in the linear approximation for any energy density of

[6] We used positive q values for the curves (86) since the Mathieu stability chart is symmetric about the a-axis.

mode $e = N/2$, so that (nongeneric) perturbations of the latter involving only these modes never lead to instability. These modes, as well as modes with $\rho > 1/3$ when $\epsilon < \epsilon_c(\rho)$, can grow only if they are triggered by the interaction with other modes that are unstable. This kind of interaction is neglected in the linear approximation around the $e = N/2$ mode, and comes into play only at later times, when unstable modes have grown and consequently the linearized theory is no longer valid.

We can now describe what happens for a given system of N particles. First of all, for $N \geq 4$ there are always modes with $\rho > 1/3$ so that the $e = N/2$ mode can never be stable for all energy densities. As ϵ_c is a decreasing function of ρ, the first modes to go unstable when ϵ is increased from zero are always $r = (N/2)-1$ and $r = (N/2)+1$, which have $\rho = \cos^2(\pi/N)$. Therefore for each (even) number N of particles there is a non-zero value $\tilde{\epsilon}(N) = \epsilon_c(\cos^2(\pi/N))$ below which the nonlinear mode $e = N/2$ is stable. In fact for $\epsilon < \tilde{\epsilon}(N)$ all the discrete points (ρ, ϵ) having abscissas (87) are below the critical curve $\epsilon_c(\rho)$ in Fig. 5. Since $\epsilon_c \to 0$ for $\rho \to 1$, the critical threshold $\tilde{\epsilon}(N)$ for the stability of the nonlinear out-of-phase mode approaches zero as the number N of particles is increased without limit. Using power series expansions of the curve in (86) and of $b_1(q)$ around the point $(q, a) = (0, 1)$, we find that $\tilde{\epsilon}(N) = \pi^2/(3N^2) + \mathcal{O}(N^{-4})$. This is in agreement with the result obtained in Ref. [46] using infinite Hill determinants. However, we do not agree with their results in Table I, which seem to indicate that low modes become unstable, while we claim that all modes with $\rho \leq 1/3$ are always stable.

Furthermore, as the ρ values (87) to be considered are increasingly dense as N is increased, for each ϵ, no matter how small, there is a value N for the system size above which the $e = N/2$ mode is unstable. In this sense, we can say that the $e = N/2$ mode is unstable at any nonzero value of the energy density in the thermodynamic limit. However for very small ϵ it mantains a metastable character, with a non-negligible lifetime, because the largest growth rate of unstable modes vanishes as $\epsilon \to 0$. This can be understood from Fig. 4 since for $k \to 0$ the unstable part of the constant k curve tends to the edge between the b_1 and a_1 lines and thus corresponds to a smaller and smaller growth rate[7].

To confirm our analysis we have numerically integrated the full nonlinear FPU model directly in normal coordinate space (Eqs. (36)). We have overcome the difficulty of the huge number of interaction terms by first calculating a table of nonzero interaction coefficient, whose number is only $\sim N^3$, which is then stored in a single vector variable with a suitable label ordering[8]. We excite mode $e = N/2$ with an energy $E_{N/2}$ corresponding to a chosen ϵ and give to all other modes an equally distributed small amount of energy, e.g. such that $\sum_{j \neq N/2} E_j / E_{N/2} \approx 10^{-13}$. Then we follow the time evolution of all the modes, observing in particular their harmonic energies. The latter are the physically

[7] We point out that our previous scalings of the time variable do not change the order of magnitude of time scales at small ϵ since $\tau \approx 2t$ for $\epsilon \to 0$.

[8] We thank J. Laskar for suggesting this trick.

relevant observables, and are observed to grow exponentially for unstable modes, while the corresponding normal coordinates oscillate with exponentially growing envelope.

First of all we have verified the scaling suggested by (82). To compare results with different N we mantain fixed the ratio $\sum_{j\neq N/2} E_j/E_{N/2}$, so that changing the N value at fixed ϵ let modes with the same r/N ratio start with the same normal coordinate amplitude. In Fig. 6 we show the modal energy spectrum at fixed time for various values of N, with the energy density associated to mode $e = N/2$ fixed at $\epsilon = 0.1$. The superposition of different spectra proves that only direct interaction between mode $e = N/2$ and other modes, through parametric excitation, is important in a first time evolution, when the only growing modes are those predicted to be unstable on the basis of the Mathieu equation stability diagram. Modes with $r/N < 0.35$ are predicted to be stable for $\epsilon = 0.1$ from the curve $\epsilon_c(\rho)$ shown in Fig. 5, in agreement with Fig. 6. We have observed that at later times stable modes begin to grow due to secondary interaction with the unstable modes grown meanwhile.

To understand the $\epsilon \to 0$ limit for the infinite chain we have numerically computed the behaviour of the fastest growth rate of the instability when ϵ is decreased while N is increased. In fact, if ϵ is decreased at fixed N, when it passes below $\tilde{\epsilon}(N)$ no instability is detected. Therefore to measure instability growth rates as ϵ decreases, we must progressively increase N. We have detected the fastest growing mode, $\bar{k}$, at each value of ϵ, and measured its exponential growth rate λ ($E_{\bar{k}} \sim 10^{\lambda t}$). The dependence of λ on ϵ, for small ϵ, can be numerically fitted with a phenomenological law $\lambda = c_1\epsilon^d + c_2$ with $d = 1.0$ $c_1 = 1.1$ and $|c_2| < 6 \times 10^{-4}$ which linearly extrapolates to a value consistent with zero in the limit $\epsilon \to 0$. We have therefore an interpretation of what might happen in the thermodynamic limit: in this limit the mode $e = N/2$ is always unstable under generic small perturbations but the rate of instability goes to zero (a sort of marginal case). It is interesting to observe that interchanging of the two limits $\epsilon \to 0$ and the thermodynamic limit $N \to \infty$ gives different answers for the stability of the $e = N/2$ mode. Stability is obtained if $\epsilon \to 0$ is performed first, while performing first the $N \to \infty$ limit we obtain instability.

An interesting and open question is the fate of the instability, since our linearized theory describes the short time scale only. For large N, the energy density stability threshold $\tilde{\epsilon}(N)$ is very small, and the $e = N/2$ mode is unstable for all relevant ϵ values. However one should still distinguish different regimes. For ϵ values large with respect to those of the instability, the system evolves towards equipartition, as it is in general known from studies on the threshold of strong stochasticity for the FPU-β system, although very little attention has been paid to high mode initial excitations, apart from Ref. [2]. However, for small ϵ, numerical results show that the (slow) growth of unstable modes saturates at later times leading to a characteristic asymptotic form of the energy spectrum where modal energies perform characteristic oscillations and recur-

rences (similar to the well known FPU recurrences present for long wavelength initial excitations). Furthermore the spectrum decays, roughly exponentially, for modes far from mode number $N/2$, and it might be possible the emergence of some coherent structure. In this connection we point out that the more unstable modes are those around the initially excited mode number, a characteristic feature of modulational instability, well studied in continuum systems such as, e.g., water waves [51]. In the context of discrete systems different from FPU models, namely chains made of *harmonically* coupled particles subjected to a nonlinear *on-site* potential, modulational instability has been proposed [52] as the first step towards the creation of states with spatially localized energy. The possible existence of spatially localized oscillations, called *intrinsic localized modes*, in FPU-type chains has been the object of much work, starting from [53], generally unrelated with studies on equipartition and energy thresholds in the same systems. Let us finally mention that in a recent interesting paper by Sandusky and Page [54], a connection is investigated between the existence of intrinsic localized modes and the instability of the "out-of-phase" mode in several kinds of one-dimensional homogeneous chains with anharmonic intersite coupling.

6 Conclusions

There has been recently a revival of interest in conservative coupled oscillator systems (see e.g. [53, 55]). In this paper we have concentrated our attention on the prototype of these systems, the Fermi-Pasta-Ulam oscillator chain [1]. Although this system has been studied for a long time, still it continues to be the source of many interesting physical problems. The first Section of this paper is devoted to a comprehensive review of old and new results (a recent historical reconstruction can be found in [56]). Then, we turn to linear mode space analysis. This was first performed in the basic paper by Izrailev and Chirikov [2], although the scope was there different. We have here derived a rather compact expression for mode coupling coefficients (see formulas (32) and (34)), which leads to an efficient writing of the Hamiltonian in mode space (see (33) and (35)). After an "intermezzo" devoted to the $N = 3$ system, where we rederive a well known integrability result by a one line proof, we pass to the central issue of the paper: the existence of low-dimensional exact soutions and invariant submanifolds. The method for proving their existence relies on a detailed analysis of mode interaction coefficients and of selection rules which prevent direct interactions among particular subsets of modes. We have thus found one-mode and two-mode integrable Hamiltonians (the latter because separable or rotation invariant) corresponding to new standing and travelling nonlinear wave solutions [see (52),(55),(62),(67), (68),(71),(73)] of the FPU system, which hold true in the thermodynamic limit. Three-mode invariant submanifolds are moreover present (see (74)), for which a Poincaré section study of two-mode associated subspaces reveals a bifurcation as the control parameter ϵ, proportional

to energy per oscillator, is varied. This bifurcation is induced by parametric perturbation and leads to the formation of stochastic layers, corresponding to intermode energy transfer. This effect suggests a physical interpretation of these bifurcations, which could be responsible for opening channels of energy transfer among modes. It should however be reminded that all submanifolds so far found correspond to high k modes. The mechanisms controlling energy transfer for low k modes seem to be completely different (see Refs. [33, 24, 30, 26]).

Moreover, the opening of a transfer channel does not necessarily mean that energy flow is completed until energy equipartition is reached; this can happen only if large-scale chaos is present, leading to the diffusion of the orbits over the whole phase space.

A complete stability analysis is possible for mode $e = N/2$, after reducing variational equations (78) to a single Lamé equation (81) and a proper interpretation of control parameters related to mode number, system size N and energy density. For finite N we prove the existence of a low energy range of stability. However this range shrinks to zero as $N \to \infty$ but, correspondingly, the rate of instability goes to zero as $\epsilon \to 0$, thus proving the presence of a sort of marginal stability of mode $e = N/2$ in the thermodynamic limit at low energy density. This is a hint to the belief that this solution might be physically relevant, and moreover encourages to look for analogous stability proofs for other one-mode and even two-mode solutions, whose existence was proven in this paper.

A more difficult matter would be the proof of stability of invariant submanifolds. The odd and even invariant submanifolds mentioned at the beginning of Section 4 also display an instability threshold. This phenomenon has been studied in connection with an instability of cnoidal waves in the modified KdV equation (mKdV) by Driscoll and O'Neil [57]; the control parameter for this instability might be different from energy density, as claimed in Ref. [24]. However the relation with this problem is not clear because the mKdV describes only the long wavelength part of the mode spectrum. The study of the stability of multi-mode invariant submanifolds will be the subject of future investigations, together with a more complete computer assisted search and classification of them.

Acknowledgments

We acknowledge useful discussions with Jayme De Luca, Giovanni Gallavotti, Allan Lichtenberg, Roberto Livi and Dima Shepelyansky. We thank the Institute for Scientific Interchange in Torino (Italy) for hospitality and use of computer facilities. This work is part of the European Network on Stability and Universality in Classical Mechanics (contract n. ERBCHRXCT940460).

References

[1] E. Fermi, J. Pasta, and S. Ulam, Los Alamos Report LA-1940 (1955), later published in *Collected Papers of Enrico Fermi*, E. Segré ed., University of Chicago Press, Chicago (1965) (Vol. II, p. 978); also reprinted in *Nonlinear Wave Motion*, A. C. Newell ed., Lect. Appl. Math. **15**, AMS, Providence, Rhode Island (1974); also in *The Many-Body Problem*, D. C. Mattis ed., World Scientific, Singapore (1993).

[2] F. M. Izrailev and B. V. Chirikov, Dokl. Akad. Nauk SSSR **166** (1966) 57 [Sov. Phys. Dokl. **11** (1966) 30].

[3] B. V. Chirikov, F. M. Izrailev, and V. A. Tayursky, Comp. Phys. Commun. **5** (1973) 11.

[4] A. N. Kolmogorov, Dokl. Akad. Nauk SSSR **98** (1954) 527; J. Moser, Nachr. Akad. Wiss. Göttingen Math. Phys. Kl. **2** (1962) 1; V. I. Arnol'd, Russ. Math. Surv. **18** (1963) 9 and 85.

[5] G. Benettin, *Ordered and Chaotic Motions in Dynamical Systems with Many Degrees of Freedom*, in *Molecular Dynamics Simulation of Statistical Mechanical Systems*, Varenna XCVII Course, G. Ciccotti and W. G. Hoover eds., North-Holland, Amsterdam (1986).

[6] R. Livi, M. Pettini, S. Ruffo, M. Sparpaglione, and A. Vulpiani, Phys. Rev. A **31** (1985) 1039; R. Livi, M. Pettini, S. Ruffo, and A. Vulpiani, Phys. Rev. A **31** (1985) 2740.

[7] H. Kantz, Physica D **39** (1989) 322.

[8] M. Pettini and M. Landolfi, Phys. Rev. A **41** (1990) 768.

[9] L. Galgani, A. Giorgilli, A. Martinoli, and S. Vanzini, Physica D **59** (1992) 334.

[10] R. Livi, A. Politi and S. Ruffo, J. Phys. A **19** (1986) 2033.

[11] J. P. Eckmann and E. Wayne, J. Stat. Phys. **50** (1988) 853.

[12] N. J. Zabusky and M. D. Kruskal, Phys. Rev. Lett. **15** (1965) 240.

[13] C. S. Gardner, J. M. Greene, M. D. Kruskal, and R. M. Miura, Phys. Rev. Lett. **19** (1967) 1095.

[14] P. D. Lax, Comm. Pure Appl. Math. **21** (1968) 467.

[15] V. E. Zakharov and L. D. Faddeev, Funct. Anal. Appl. **5** (1971) 280.

[16] M. J. Ablowitz, D. J. Kaup, A. C. Newell, and H. Segur, Phys. Rev. Lett. **31** (1973) 125.

[17] M. J. Ablowitz and H. Segur, *Solitons and the Inverse Scattering Transform*, SIAM, Philadelphia (1981); M. J. Ablowitz and P. A. Clarkson, *Solitons, Nonlinear Evolution Equations and Inverse Scattering*, Cambridge University Press (1991).

[18] G. Benettin, G. Lo Vecchio, and A. Tenenbaum, Phys. Rev. A **9** (1979) 1252; G. Benettin, A. Tenenbaum, Phys. Rev. A **28** (1983) 3020.

[19] L. Casetti, R. Livi, A. Macchi, and M. Pettini, *Relaxation times in an anharmonic crystal with diluted impurities*, submitted to Europhysics Letters (1994).

[20] J. L. Tuck, Los Alamos Report LA-3990 (1968); J. L. Tuck and M. T. Menzel, Adv. Math. **9** (1972) 399.

[21] D. Ruelle, Commun. Math. Phys. **87** (1982) 287.

[22] P. Manneville, in *Macroscopic Modeling of Turbulent Flows*, O. Pironneau ed., Lecture Notes in Physics **230**, 319, Springer-Verlag, Berlin (1985).

[23] Ya. G. Sinai, *A remark concerning the thermodynamical limit of Lyapunov spectrum*, preprint (1995).

[24] J. De Luca, A. J. Lichtenberg, and M. A.Lieberman, Chaos **5** (1995) 283.

[25] H. Kantz, R. Livi and S. Ruffo, J. Stat. Phys. **76** (1994) 627.

[26] J. De Luca, A. J. Lichtenberg, and S. Ruffo, Phys. Rev. E **51** (1995) 2877.

[27] M. Pettini, Phys. Rev. E **47** (1993) 838; L. Casetti and M. Pettini, Phys. Rev. E **48** (1993) 4320.

[28] L. Casetti, R. Livi, and M. Pettini, Phys. Rev. Lett. **74** (1995) 375.

[29] N. N. Nekhoroshev, Funct. Anal. Appl. **5** (1971) 338; Russ. Math. Surv. **32** (1977) 1.

[30] F. Fucito, F. Marchesoni, E. Marinari, G. Parisi, L. Peliti, S. Ruffo, and A. Vulpiani, J. de Physique **43** (1982) 707.

[31] R. Livi, M. Pettini, S. Ruffo, M. Sparpaglione, and A. Vulpiani, Phys. Rev. A **28** (1983) 3544.

[32] D. L. Shepelyansky, unpublished (1994).

[33] P. Poggi, S. Ruffo, and H. Kantz, Phys. Rev. E **52** (1995) 307.

[34] B. V. Chirikov, Phys. Rep. **52** (1979) 263.

[35] J. Ford, J. Math. Phys. **2** (1961) 387; J. Ford and J. Waters, J. Math. Phys. **4** (1963) 1293; E. A. Jackson, J. Math. Phys. **4** (1963) 551 and 686.

[36] D. S. Sholl and B. I. Henry, Phys. Lett. A **159** (1991) 21.

[37] B. I. Henry and J. Grindlay, Physica D **28** (1987) 49.

[38] N. Ooyama, H. Hirooka, and N. Saito, J. Phys. Soc. Japan **27** (1969) 815; N. Saito, N. Ooyama, Y. Aizawa, and H. Hirooka, Suppl. Prog. Theor. Phys. **45** (1970) 209; N. Saito, N. Hirotomi, and A. Ichimura, J. Phys. Soc. Japan **39** (1975) 1431.

[39] R. L. Bivins, N. Metropolis, and J. R. Pasta, J. Comp. Phys. **12** (1973) 65.

[40] D. Sholl, Phys Lett. A **149** (1990) 253.

[41] D. S. Sholl, *Analytic Methods for Nonlinear Lattices*, Bachelors thesis, The Australian National University (1991).

[42] G. V. Choodnovsky and D. V. Choodnovsky, Lettere al Nuovo Cimento **19** (1977) 291.

[43] D. F. Lawden *Elliptic Functions and Applications*, Springer-Verlag, New York (1989).

[44] *Handbook of Mathematical Functions*, M. Abramowitz and I. A. Stegun eds., Dover, New York (1965).

[45] M. Toda, Phys. Rep. **18** (1975) 1.

[46] N. Budinsky and T. Bountis, Physica D **8** (1983) 445.

[47] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis*, 4th ed., Cambridge University Press, Cambridge (1946).

[48] F. M. Arscott, *Periodic Differential Equations*, Pergamon (1964).

[49] W. Magnus and S. Winkler *Hill's Equation*, Interscience, New York (1966).

[50] G. Pecelli and E. S. Thomas, Quart. Appl. Math. **36** (1978) 129.

[51] T. B. Benjamin and J. E. Feir, J. Fluid Mech. **27** (1967) 417.

[52] Y. S. Kivshar and M. Peyrard, Phys. Rev. A **46** (1992) 3198; T. Dauxois and M. Peyrard, Phys. Rev. Lett. **70** (1993) 3935.

[53] A. S. Dolgov, Sov. Phys. Solid State **28** (1986) 907; A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61** (1988) 970; J. B. Page, Phys. Rev. B **41** (1990) 7835.

[54] K. W. Sandusky and J. B. Page, Phys. Rev. B **50** (1994) 866.

[55] R. S. MacKay, S. Aubry, Nonlinearity **7** (1994) 1623.

[56] J. Ford, Phys. Rep. **213** (1992) 271.

[57] C. F. Driscoll and T. M. O'Neil, Phys. Rev. Lett. **37** (1976) 69; Rocky Mountain J. of Math. **8** (1978) 211.

Figure captions

Fig. 1. Poincaré section for the system (75) on the $(Q_{N/4}, P_{N/4})$ plane, with $\beta/N = 0.4$. The energy value E corresponds to $\epsilon = \beta E/N = 1.0$. Each smooth curve corresponds to a different initial condition on the constant energy shell. The fixed point at the origin, representing the periodic oscillation (52) on the lattice, is stable.

Fig. 2. Poincaré section for the system (75) on the $(Q_{N/4}, P_{N/4})$ plane, with $\beta/N = 0.4$. The energy value E corresponds to $\epsilon = \beta E/N = 1.25$. The fixed point at the origin has become unstable and a pair of new stable fixed points has bifurcated from it (see text for details).

Fig. 3. Poincaré section for the system (75) on the $(Q_{N/4}, P_{N/4})$ plane, with $\beta/N = 0.4$. The energy value E corresponds to $\epsilon = \beta E/N = 10.0$. The fixed point at the origin, which is by now unstable, lies within a stochastic layer.

Fig. 4. Stability chart of the Mathieu equation (85). The instability region lies between the continuous lines. $b_1(q)$ is the lower bound and $a_1(q)$ the upper one. The lines match at $(0, 1)$. We draw in the figure also the (q, a) lines in formula (86), parametrized by ρ and k. The dashed lines correspond to a fixed ρ and a continuosly varying k from 0 to $1/\sqrt{2}$; they are traced at ρ intervals of 0.1 from $\rho = 0$ to $\rho = 0.9$. The dotted lines correspond instead to a fixed k and a continuously varying ρ from zero to one; the curves are traced at k^2 intervals of 0.05 from 0.05 to 0.5. Crossings of the lines in formula (86) with the $b_1(q)$ line correspond to transitions to instability.

Fig. 5. Marginal stability curve $\epsilon_c(\rho)$ (full line). The vertical asymptote at $\rho = 1/3$ (dotted) is also traced to mark the fact that all modes with $\rho < 1/3$ are stable for any ϵ value.

Fig. 6. Modal linear energies E_r vs. the ratio of the mode number r to the system size N at fixed time $t = 30$. Different symbols correspond to different system sizes: $(+)$ $N = 8$; $(\times)$ $N = 16$; $(\Box)$ $N = 32$; $(\diamond)$ $N = 64$. The continuous curve is an interpolation to guide the eyes. The initial values of modal energies are 3.2×10^{-13}.